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Generalized oscillator strengths for the $3s\,^2S \rightarrow 3p\,^2P$ transition in Mg II

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Generalized oscillator strengths (GOS's) are calculated from accurate five-state close-coupling differential cross sections for the resonance transition in Mg II at electron impact energies 15, 50, 60, and 100 eV. Curves of the GOS versus momentum transfer squared, K^2, remain separate down to zero scattering angle, with the 50, 60, and 100 eV curves showing maxima close to $K^2=0$. We interpret the new phenomenon, maxima at small scattering angles, as a manifestation of the inadequacy of the Lassettre, Skerbele, and Dillon formula to represent the GOS at small K^2 for intermediate energies. At 50 eV our GOS's compare well with those deduced from measurement.

INTRODUCTION

Electron impact excitation of atoms and ions is important among other things in the design and feasibility of new lasers and tokamak-type plasmas. In particular, Mg II lines are better diagnostic of solar and stellar atmospheres.[1,2] Apart from guiding the first differential-cross-section measurement for inelastic excitation of an ion by electron impact,[3] accurate theoretical differential cross sections have been used to resolve[4] most of the discrepancy between experiment and calculation for the $4p\,^2P^0$ cross section of Cu. Agreement with experiment was achieved by normalizing the generalized oscillator strength (GOS) curves deduced from the data of Trajmar, Williams, and Srivastava[5] to the close-coupling GOS's. Also, experimental and theoretical differential cross sections for excitation of the resonance transition in Mg II have been obtained.[6]

Lassettre, Skerbele, and Dillon[7] have deduced that a GOS curve for an electron impact excitation process converges to the optical oscillator strength as $K^2 \rightarrow 0$. Further, they inferred that their result should be valid for inelastic electron transitions irrespective of the applicability of the Born approximation and at any energy. The limiting behavior of the GOS as $K^2 \rightarrow 0$ is important *inter alia* in the normalization of the experimentally determined relative differential cross sections[8,9] for excitation of atoms by electron impact and calculation of cross sections for energy transfer.[11]

Several investigations[10–17] have examined the behavior of the GOS near $K^2=0$. No clear departures from the limit theorem have been reported. However, Klump and Lassettre[15] have communicated difficulties in extrapolating the GOS to the optical oscillator strength. Recently, contradictions to the expected limiting behavior of GOS curves have been found[4,18] in resonance transitions for Cu and Zn II by electron impact.

Normal trends are demonstrated for the limiting behavior[16,17] of the GOS vs K^2 for Hg as $K^2 \rightarrow 0$. Near their minima, GOS curves for Hg separate with kinetic energy and then converge to a single curve as $K^2 \rightarrow 0$. The separation of the curves is a manifestation of the failure of the first Born approximation.[16,17] As $K^2 \rightarrow 0$ the GOS curves appear to merge to a single curve which apparently approaches $K^2=0$ smoothly and monotonically, indicating the applicability of the first Born approximation well below the region of minima. From the measurements two significant features are evident: (i) in the region of the minima of the GOS, the Born approximation has no validity and (ii) as $K^2 \rightarrow 0$, it appears that the limit theorem of Lassettre *et al.*[7] is being confirmed by the measurements.

THEORY

In the Born approximation, the GOS, $f_{0n}^G(K)$ is related to the Born differential cross section, $(d\sigma/d\Omega)_{0n}^B$ by[19,20]

$$f_{0n}^G=\frac{W}{2}\frac{k_0}{k_n}K^2\left(\frac{d\sigma}{d\Omega}\right)_{0n}^B \ , \tag{1}$$

where

$$K^2=2E(2-W/E-2\sqrt{1-W/E}\,\cos\theta) \ . \tag{2}$$

W, k_0, and k_n are the excitation energy and the electron momenta before and after collision, K and θ are the momentum transfer and the scattering angle, and E is the total energy of the system.

Lassettre *et al.*[7] have derived the limit theorem on the apparent generalized oscillator strength

$$\lim_{K\rightarrow 0} f_{0n}^G(K)=f \ , \tag{3}$$

where f is the optical oscillator strength. They claim that Eq. (3) must hold for collision processes at any energy even when the first Born approximation is not applicable. Clearly, at $K^2=0$, $f_{0n}^G(K)=f$. The problem is then the manner in which the limit is approached. That is what the Lassettre *et al.* "limit theorem" is about.

In practical application of Eq. (1), $(d\sigma/d\Omega)_{0n}^B$ is replaced by the experimentally determined value $(d\sigma/d\Omega)_{0n}^E$. Normalization of the measured relative differential cross sections is then effected through use of Eq. (3). In our theoretical investigation we replace in Eq. (1) $(d\sigma/d\Omega)_{0n}^B$ by the accurate multistate close-coupling value. Since our differential cross sections are absolute, the calculated $f_{0n}^G(K)$ are also absolute. Thus our GOS can provide a

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good procedure for normalizing measured differential cross sections.

Here we communicate results of our investigation of dominant features in $f_{0n}^G(K)$ vs K^2 curves in the region of small K^2. The $3s\,^2S \rightarrow 3p\,^2P^0$ transition in Mg II is selected because accurate multistate close-coupling differential cross sections and measurements are available. The investigation is carried out at 15, 60, and 100 eV electron impact energies, and at 50 eV because experimental data are available.[6] The objective is to study the limiting behavior of the GOS for inelastic excitation at small K^2 values and its compatibility with the limit theorem.[7]

In determining whether $f_{0n}^G(K)$ given by Eq. (1) approaches the optical oscillator strength as $K^2 \rightarrow 0$ for inelastic scattering, we have to consider two important issues. (1) There is no theory that prescribes the extrapolation of $f_{0n}^G(K)$ from the smallest $K^2(\theta=0)$ through the unphysical region to $K^2=0$. (2) Equation (1) was obtained assuming the validity of the first Born approximation. To be consistent with the limit theorem, our GOS vs K^2 curves for various primary energies must converge to a single curve as $K^2 \rightarrow 0$ which can then be extrapolated readily and unambiguously to the optical oscillator strength. However, should the GOS vs K^2 curves remain separated with energy or show structure in the region $K^2 \rightarrow 0$, we may conclude that $f_{0n}^G(K)$ is inadequately represented by Eq. (1) for small K^2 values. Then the latter ceases to be useful for normalization of experimentally determined differential cross sections.

RESULTS

In our calculation of the GOS, we replace $(d\sigma/d\Omega)_{0n}^B$ in Eq. (1) by the five-state close-coupling approximation differential cross section for Mg II.[21] The values for W and f are 0.16 a.u. and 0.97, respectively, and were obtained from our target wave function. Both agree well with accepted values. Details of the calculation of the differential cross sections are given elsewhere.[21] The theoretical value for W was also used for calculating GOS from the experimental data.

Figure 1 shows $f_{0n}^G(K)$ against K^2 for values of $E=15$, 60, and 100 eV. Note the progressive movement of the position of the minima to smaller values of K^2 as E decreases (minimum of 100 eV curve is not shown but is closer to $K^2=2.0$ a.u.). As $K^2 \rightarrow 0$, the various GOS curves appear to be converging to a single curve which can be extrapolated unambiguously to the optical f value, $f=0.97$. Thus far the behavior is typical and has also been observed and discussed for Hg.[16,17]

Figure 2 shows $f_{0n}^G(K)$ vs K^2 in the range $0\text{ a.u.} \leqslant K^2 \leqslant 0.28$ a.u. The vertical scale is now linear. The curves remain distinctly separated with energy down to $\theta=0$, except for the fortuitous merging of the 15 and 60 eV curves at $K^2=0.027$ a.u. The 60 and 100 eV curves show maxima near $K^2=0$. Neither the 60 nor the 100 eV curve can be extrapolated smoothly and monotonically to the optical f value. The maxima near $K^2=0$ are new features and are due to structure in $K^2(d\sigma/d\Omega)$ for small physical K^2.

In the region of interest here ($0 \leqslant \theta \leqslant 20°$, away from the diffraction maxima and minima of $d\sigma/d\Omega$), $d\sigma/d\Omega$ has no structure[22] and is rapidly decreasing with θ while K^2 is in-

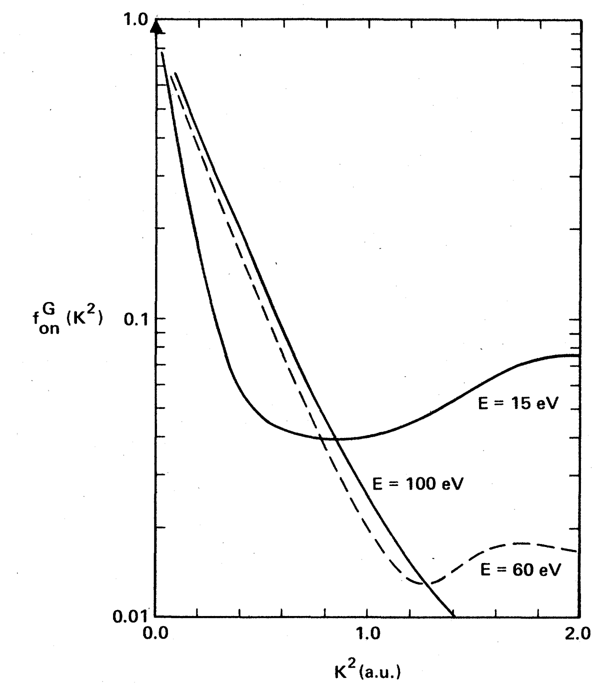

FIG. 1. $f_{0n}^G(K^2)$ vs K^2 for the $3s\,^2S \rightarrow 3p\,^2P^0$ transition of Mg II at $E=15$, 60, and 100 eV. Note the log scale for the $f_{0n}^G(K^2)$ axis. ▲ = 0.97 represents the optical f value.

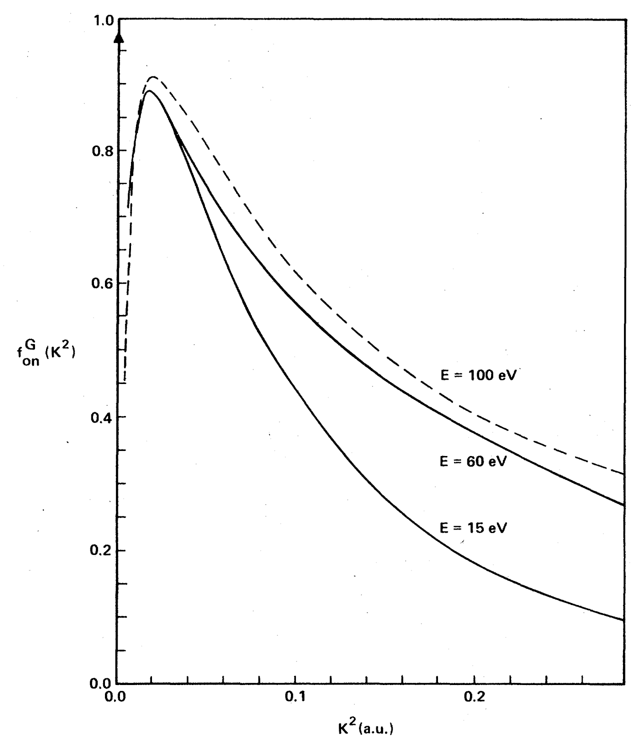

FIG. 2. $f_{0n}^G(K^2)$ against K^2 in the range $0 \leqslant K^2 \leqslant 0.28$ a.u., showing the maxima for $E=60$ and 100 eV curves near $K^2=0$. The curves are separated in energy down to $\theta=0$. At $\theta=0$, the 15 eV curve does not overlap the 60 eV curve as the lines appear to suggest.

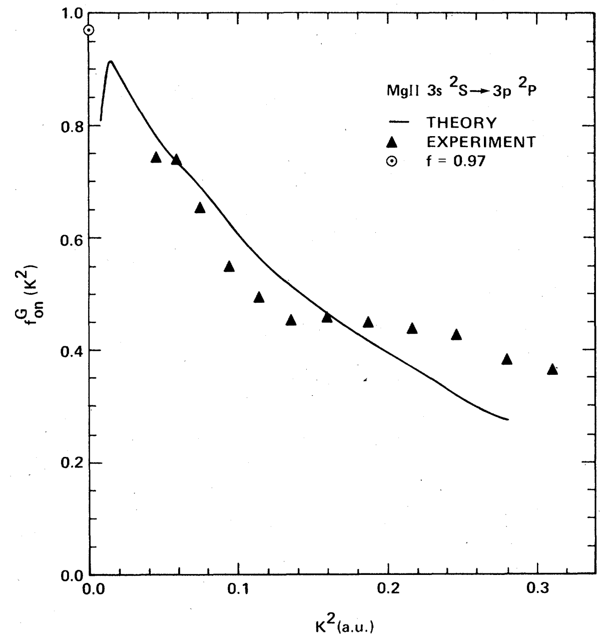

FIG. 3. Comparison between calculated (solid curve) and experimental (solid triangles) $f_{0n}^G(K^2)$ against K^2 at 50 eV. The circle represents the optical f value.

creasing with θ. Further, there is no particularly dominant partial wave that contributes to the cross sections. The main contribution to the cross sections is spread over a range of several partial waves in all the energies considered in this paper. For example, the lower limit starts near $L=3$ (L is the orbital angular momentum) at 15 eV and rises to near $L=8$ at 100 eV with the corresponding spread in L being roughly 5 and 10, respectively.

Figure 3 compares theoretical GOS's with those deduced from measurement[6] at 50 eV. Comparison between theory and measurement could be effected only for values of K^2 corresponding to $\theta \geq 6°$. Experimental difficulties prevent measurement of the differential cross sections for $0 \leq \theta < 6°$. Like in the 60 and 100 eV curves, a maximum is evident in the theoretical curve near $K^2=0$ and is due to structure in $K^2(d\sigma/d\Omega)$. Agreement in shape between the theoretical curve and experimental data is reasonable in the angular range $6° \leq \theta \leq 13°$ (0.046 a.u. $\leq K^2 \leq 0.187$ a.u.). Experimental differential cross sections were normalized to those from theory at 12°. Their flattening[6] around 12–15° translates into a minimum in the GOS which is absent in the calculated curve. The flattened differential cross section in the original experimental data could not be explained.[6]

A remark regarding the accuracy of our calculation is appropriate. The differential cross sections used to calculate the GOS are accurate. They are multistate close-coupling differential cross sections obtained with the use of good configuration-interaction wave functions. They have checked very well with measurements,[6] including integral cross sections.[21] Maxima for GOS curves near $K^2=0$ have been reported for Cu.[4] The GOS from the differential-cross-section measurements for excitation of Na $3p\,^2P$ at 54.4 eV by Shuttleworth, Newell, and Smith[23] also indicates a maximum near $K^2=0$. Interestingly, GOS's calculated from our multistate close-coupling differential cross sections for the forbidden transitions (obtained simultaneously with those for the resonance transitions) in Cu, Zn II, and Mg II *all* are consistent with the Lassettre *et al.* limit theorem.

DISCUSSION AND CONCLUSION

If the expression for $f_{0n}^G(K)$ given by Eq. (1) remains applicable for inelastic scattering at small and intermediate impact energies, then our results for Mg II suggest interesting physics at small scattering angles. However, since the first Born approximation was used to derive Eq. (1), we believe that our results are rather a manifestation of the nonapplicability of the formula for $f_{0n}^G(K)$ to resonance scattering at small and intermediate energies. The predicted maxima near $K^2=0$ in the GOS due to the structure in $K^2(d\sigma/d\Omega)$ may well be an artifact of the theory, i.e., Eq. (1). Whatever interpretation is assigned to the origin of the GOS maxima near $K^2=0$, it is clear that the use of Eq. (1), without reliable theoretical results, to normalize the experimentally determined differential cross sections may lead to serious errors.

In conclusion, we suggest that the Born series be examined more carefully and that differential cross sections for atoms and ions be measured accurately near zero scattering angles at intermediate energies to throw a deeper insight into the behavior of the GOS near $K^2 \rightarrow 0$. Our GOS's agree in shape reasonably well with measurement at 50 eV for 0.046 a.u. $\leq K^2 \leq 0.187$ a.u.

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[1]P. Lemaire, M. Choucq-Bruston, and J. C. Vial, Sol. Phys. **90**, 63 (1984).

[2]P. Lemaire and P. Gouttebroze, Astron. Astrophys. **125**, 241 (1983).

[3]A. Chutjian, A. Z. Msezane, and R. J. W. Henry, Phys. Rev. Lett. **50**, 1357 (1983).

[4]A. Z. Msezane and R. J. W. Henry, Phys. Rev. Lett. (to be published).

[5]S. Trajmar, W. Williams, and S. K. Srivastava, J. Phys. B **10**, 3323 (1977).

[6]I. D. Williams, A. Chutjian, A. Z. Msezane, and R. J. W. Henry, Astrophys. J. (to be published).

[7]E. N. Lassettre, A. Skerbele, and M. A. Dillon, J. Chem. Phys. **50**, 1829 (1969).

[8]L. Vuskovic, S. Trajmar, and D. F. Register, J. Phys. B **15**, 2517 (1982).

[9]L. Vuskovic, L. Maleki, and S. Trajmar, J. Phys. B **17**, 2519 (1984).

[10]I. V. Hertel and K. J. Ross, J. Phys. B **2**, 285 (1969).

[11]K. N. Klump and E. N. Lassettre, J. Chem. Phys. **68**, 3511 (1978).

[12]K. N. Klump and E. N. Lassettre, J. Chem. Phys. **68**, 886 (1978).
[13]A. Skerbele and E. N. Lassettre, J. Chem. Phys. **55**, 424 (1971).
[14]E. N. Lassettre, J. Chem. Phys. **43**, 4479 (1965).
[15]K. N. Klump and E. N. Lassettre, Chem. Phys. Lett. **51**, 99 (1977).
[16]F. Hanne and J. Kessler, Phys. Rev. A **5**, 2457 (1972).
[17]A. Skerbele and E. N. Lassettre, J. Chem. Phys. **58**, 2887 (1973).
[18]A. Z. Msezane and R. J. W. Henry, Chem. Phys. Lett. **119**, 81 (1985).
[19]H. A. Bethe, Ann. Phys. (Leipzig) **5**, 325 (1930).
[20]M. Inokuti, Rev. Mod. Phys. **43**, 297 (1971).
[21]A. Z. Msezane and R. J. W. Henry (unpublished).
[22]A. Z. Msezane and R. J. W. Henry, Phys. Rev. A (to be published).
[23]T. Shuttleworth, W. R. Newell, and A. C. H. Smith, J. Phys. B **10**, 1641 (1977).