Generalized oscillator strengths for dipole-forbidden transitions in Cu I, Zn II, and Mg II

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Accurate electron-impact differential cross sections for various optically forbidden transitions in Cu I, Mg II, and Zn II are used to calculate apparent generalized oscillator strengths (GOS's) in the electron-impact energy range $15 \le E \le 100$ eV. Most curves of the GOS versus momentum transfer squared, K^2, appear compatible with the Lassettre-limit theorem. Extrapolation to the optical oscillator strength values is meaningless for the 15-eV curves of Mg II and Zn II for which the unphysical region is significant. The GOS minima, where they exist, near $K^2 \rightarrow 0$ are extremely important in assessing whether a given transition is interpretable in terms of the Born approximation.

INTRODUCTION

Electron-impact excitation cross sections for atoms and ions are important in such diverse fields as high-temperature plasmas in laboratory and astrophysical systems, laboratory fusion plasmas, and lasers. Differential cross sections which are very sparse for ions provide a stringent test of theoretical calculations when they are compared with measurements. The difficulty of the measurements of the excitation cross section, both differential and integral, necessitates the implementation of reliable calculational procedures applicable to various collision systems to guide measurements.

Relative differential electron-impact cross sections have been measured and contrasted for the resonance and the first optically forbidden transitions in Mg II, Zn II, and Cd II.[1] Mg II lines are better diagnostic of solar and stellar atmospheres[2,3] and Cu I is a potential laser material.[4] Multistate close-coupling (CC) differential cross sections have guided the first measurement[5] for inelastic excitation of an ion by electron impact and used to resolve most of the discrepancy between experiment and calculation for Cu I.[6] CC differential cross sections have also been calculated and contrasted for Cu I, Zn II, and Mg II.[7] The need for the transformation of the measured relative cross sections to absolute cross sections and for a deeper understanding of excitation as the nuclear charge increases from low to high Z values have generated increasing interest in small-angle inelastic electron scattering at low and moderate impact energies.

Particularly interesting is the theoretical investigation using multistate CC differential cross sections of the limiting behavior of the generalized oscillator strength (GOS) as $K^2 \rightarrow 0$. The GOS concept has been suggested for use in converting the measured relative differential cross sections to absolute values, through Lassettre's limit theorem,[8] which established the connection between electron impact spectroscopy and optical spectroscopy, using optical oscillator strengths. The reason is that the latter are readily available for many dipole allowed transitions of ions and atoms; whereas reliable theoretical differential cross sections are generally difficult to obtain. Recently, the GOS procedure has suffered a serious drawback. Resonance transitions in Cu I,[6] Mg II,[9] and Na I,[10] reveal GOS's that are incompatible with the Lassettre limit theorem,[8] particularly at small values of E.

In this paper we compare and contrast the GOS versus K^2, at small values of K^2, for optically forbidden transitions in Cu I, Mg II, and Zn II. The purpose is to assess the applicability of the GOS concept to optically forbidden transitions near $K^2 \rightarrow 0$ at small and moderate E values. To calculate the GOS, we use the multistate close-coupling differential cross sections for forbidden transitions which were obtained simultaneously with the resonance differential cross sections, which have been used already to test the Lassettre limit theorem. The present calculation is therefore at the same level of accuracy as our previous resonance results.

For Mg II the five states $3s\,^2S$, $3p\,^2P^\circ$, $3d\,^2D$, $4s\,^2S$, and $4p\,^2P^\circ$ were coupled. In the case of Cu I and Zn II, four states were employed, coupling the $4s\,^2S$, $3d^9 4s^2\,^2D$, $4p\,^2P^\circ$, and $5s\,^2S$, and the $4s\,^2S$, $4p\,^2P^\circ$, $3d^9 4s^2\,^2D$, and $4d\,^2D$ states, respectively.

THEORY

The GOS $f_{on}^G(K)$ is related to the Born differential cross section, $(d\sigma/d\Omega)_{on}^B$ by[11,12] [atomic units (a.u.) are used throughout]

$$f_{on}^G = (\Delta E/2)(k_o/k_n)K^2(d\sigma/d\Omega)_{on}^B \ , \qquad (1)$$

where

$$K^2 = 2E[2 - \Delta E/E - 2(1-\Delta E/E)^{1/2}\cos\theta] \ . \qquad (2)$$

ΔE, k_0, and k_n are the excitation energy and the elec-

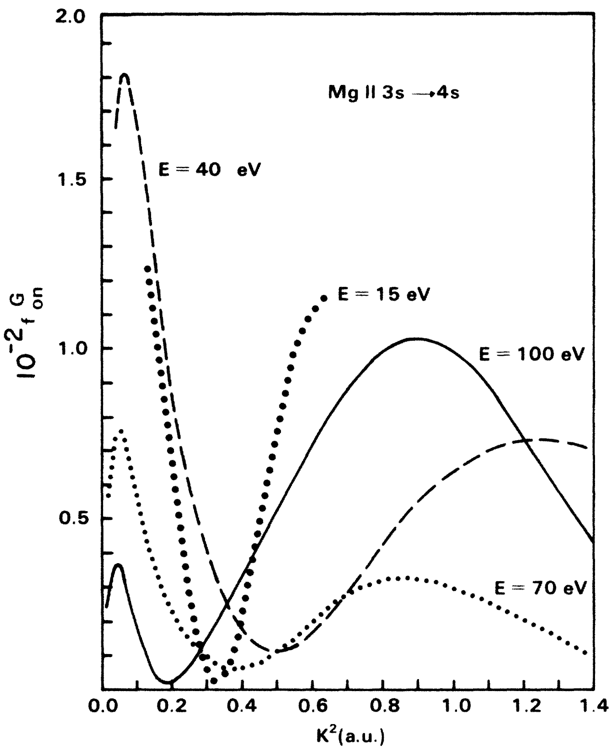

FIG. 1. Apparent generalized oscillator strength, f^G_{on} versus momentum transfer squared, K^2 (a.u.), for the optically forbidden Mg II $3s \rightarrow 4s$ transition. The curves in the figure are 15 (····), 40 (— — —), 70 (· · · ·), and 100 eV (——) impact energies.

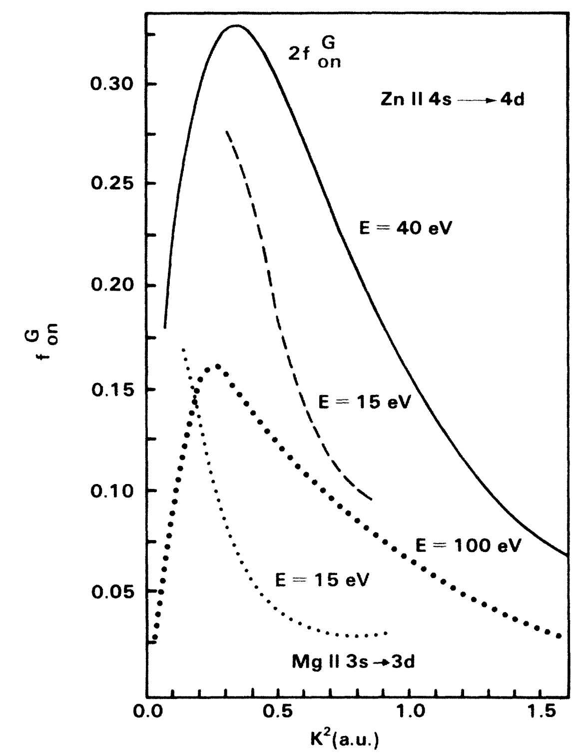

FIG. 2. f^G_{on} against K^2 (a.u.) for the Zn II $4s \rightarrow 4d$ transition: 15 (— — —), 40 (——), and 100 eV (····); and the Mg II $3s \rightarrow 3d$ transition: 15 eV (· · · ·).

tron momenta before and after collision, K and θ are the momentum transfer and the scattering angle. E is the total energy of the system.

Lassettre *et al.*[8] have derived the limit theorem on the GOS

$$\lim_{K \to 0} f^G_{on}(K) = f \ , \tag{3}$$

where f is the optical oscillator strength. They claim that Eq. (3) must hold for collision processes at any energy irrespective of the applicability of the Born approximation. Clearly, at $K^2=0$, $f^G_{on}(K)=f$. A major problem, however is the manner in which the limit is approached and how to effect extrapolation through the unphysical region to $K^2=0$.

In practical application of Eq. (1), $(d\sigma/d\Omega)^B_{on}$ is replaced by the experimentally determined value $(d\sigma/d\Omega)_{on}$. Normalization of the measured relative differential cross sections is then achieved through the use of Eq. (3). Vuskovic, Trajmar, and Register[13] have discussed the difficulty associated with the practical implementation of Eq. (3). In our theoretical investigation of the limit theorem, we replaced in Eq. (1) $(d\sigma/d\Omega)^B_{on}$ by the calculated multistate close-coupling values. Since our differential cross sections are absolute, the calculated $f^G_{on}(K)$ are also absolute. Thus our close-coupling differential cross sections can provide a good test of the applicability of the limit theorem to ionic species, transition processes, and collision energies.

RESULTS

Figure 1 shows f^G_{on} versus K^2 (a.u.) for the Mg II $3s \rightarrow 4s$ transition at $E=15$, 40, 70, and 100 eV. The well-known minima[12] in the GOS are evident. Their magnitudes have nonzero values as expected, suggesting incompatibility of the transition at the energies with the Born approximation. Note that the 15-eV curve has a deeper minimum compared to the 40- or 70-eV curve, and that the various curves fail, contrary to conventional wisdom, to merge to a single curve as $K^2 \rightarrow 0$. The 15-eV curve extrapolates to a value for $f \neq 0$ which is completely wrong. Its interpretation on the basis of the Born approximation would be completely erroneous. As E increases from 40 to 100 eV the value of the maximum decreases, the minimum becomes deeper, and the termination point of the GOS approaches the f^G_{on} axis, consistent with the Lassettre limit theorem for dipole-forbidden transitions.

Figure 2 shows the GOS against K^2 for the Zn II $4s \rightarrow 4d$ transition at 15, 40, and 100 eV. Also displayed is the GOS for the Mg II $3s \rightarrow 3d$ transition at 15 eV. The behavior of the Zn II curves is essentially the same as for the Mg II $3s \rightarrow 4s$ transition. For the 40- and 100-

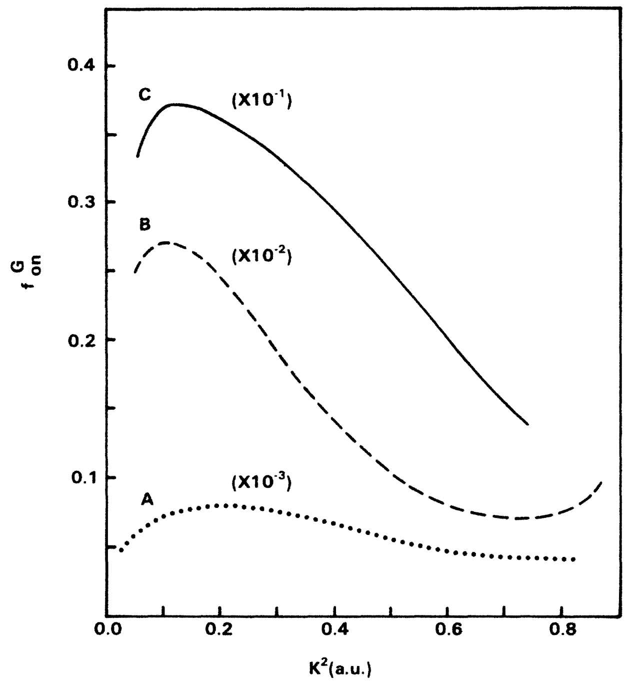

FIG. 3. Curves A and B are results for f_{on}^{G} vs K^2 (a.u.) for the dipole forbidden transition as $4s \rightarrow 3d^9 4s^2$ of Zn II at 100 and 50 eV, respectively. Curve C represents the result for the dipole forbidden Zn II $4s \rightarrow 5s$ transition at 50 eV.

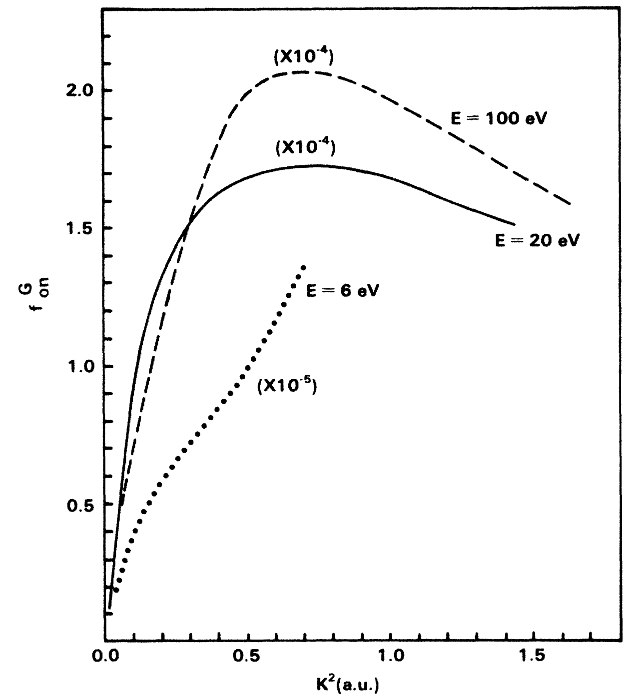

FIG. 4. The data is for the Cu I $4s \rightarrow 3d^9 4s^2$ transition: 20 (——), 60 (····), and 100 eV (— — —).

eV curves, the positions of the minima (not shown) are roughly at $K^2 \sim 2$ a.u. Here also, the minima have nonzero values; more so than in the case of the Mg II $3s \rightarrow 4s$ transition. Even at 100 eV the Born region has not yet been realized. This is consistent with the observation[12] that any deviation of the minima from the exact zero measures the departure from the first Born approximation. Both the 15-eV curves exhibit strong non-Born behavior, and their extrapolation, using whatever formula, leads to a completely wrong f value.

Plots A and B in Fig. 3 give f_{on}^{G} versus K^2 for the dipole-forbidden transition $4s \rightarrow 3d^9 4s^2$ of Zn II at 100 and 50 eV, respectively; curve C represents the result for the Zn II $4s \rightarrow 5s$ transition at 50 eV. Curve B shows a minimum at about $K^2 = 0.75$ a.u. and a maximum near $K^2 = 0.11$ a.u. For curve A the magnitude of the maximum has decreased, the minimum has almost disappeared and the overall curve has flattened and decreased by about an order of magnitude compared to curve B. Curve A has the interesting feature that its nonzero value minimum is a manifestation of the inappropriateness of the description of the excitation process in terms of Born approximation even at this high an energy. Kim and Cheng[14] arrived at a similar conclusion for Na. The unphysical regions for curves B and C are significant for comfortable simple extrapolation to $K^2 = 0$.

Figure 4 gives the results for the Cu I $4s \rightarrow 3d^9 4s^2$ transition. All appear to be consistent with the Lassettre limit theorem. Note, however, that the 100-eV curve of Cu I differs considerably from that of Zn II. In Cu I the $3d^9 4s^2$ level is below the $4p$ and in Zn II the two levels are reversed and, thus have quite different ΔE values in either system. The 100-eV curve extrapolates readily to $K^2 = 0$ since the unphysical region in this case is small. The last value of K^2, corresponding to the greatest value of f_{on}^{G} for the 6-eV curve, is evaluated at a fairly large scattering angle, $\sim 85°$, in comparison with the 20- and 100-eV curves.

SUMMARY AND CONCLUSION

For the Mg II $3s \rightarrow 4s$ optically forbidden transition, the characteristic minima for the GOS are evident. Their departure from exact zero value is a manifestation of the inapplicability of the first Born approximation to the transition at the impact energies considered here. The deeper minimum by comparison with the others exhibited by the 15-eV curve is fortuitous. The Mg II $3s \rightarrow 4s$, the Mg II $3s \rightarrow 3d$, and the Zn II $4s \rightarrow 4d$ transitions at 15 eV all are strongly non-Born, have significant unphysical regions, and their GOS's cannot be extrapolated to the optical oscillator strength. The Cu I $4s \rightarrow 3d^9 4s^2$ transition curves appear compatible with the Lassettre limit theorem, even, surprisingly, the 6-eV curve.

We conclude by noting that the minima, where they exist near $K^2 \rightarrow 0$, are extremely useful in assessing whether a given transition at a given E is interpretable in terms of the Born approximation. Therefore, except for the Cu I results, most of the transitions at the energies considered here are strictly non-Born type since their corresponding minima in the region $K^2 \rightarrow 0$ deviate from exact zero values. Also, the present data and the resonance results[9] for Mg II bring into focus the question, first raised by Huo[15] and again addressed recently by Bonham and Gorucanthu,[16] concerning the limiting slope $(df_{on}^{G}/dK^2)_{K=0}$. According to Huo,[15] for dipole-allowed transitions it becomes infinite at all finite impact energies and does not obey the Born approximation. Needless to say, that confusion abounds here, and what is needed is a careful theoretical investigation of the GOS as $K^2 \rightarrow 0$ outside the Born approximation approach. We believe that analysis of the limiting behavior of the GOS as $K^2 \rightarrow 0$ at small and moderate energies, using the latter approximation, may not lead to a better understanding; but rather to more confusion. Finally, it is hoped that the varied results of this paper representing different atomic and ionic transitions at selected small and intermediate electron impact energies manifest some possibilities for optically forbidden transitions.

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