

## Generalized oscillator strengths for inner-shell electron transitions

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A second-quantization formalism has been used to obtain a general expression for the generalized oscillator strength (GOS) for inner-shell electron transitions between two open shells of any atom. The present formula together with the spin polarized technique of the random-phase approximation with exchange are then employed to investigate correlation effects in the GOS for the Na  $2p^63s(^2S) \rightarrow 2p^53s^2(^2P)$  transition. Results are compared with those measured by Bielschowsky *et al.* [Phys. Rev. A **43**, 5975 (1991)]. The present formula has also been used with Hartree-Fock wave functions to calculate the GOS's for the carbon  $2s^22p^2(^3P) \rightarrow 2s2p^3(^3P)$  and  $2s^22p^2(^3P) \rightarrow 2s2p^3(^3D)$  transitions. The calculated multiplet oscillator strengths for the two transitions are compared with the experimental values.

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### I. INTRODUCTION

The generalized oscillator strength (GOS), first introduced by Bethe [1] to describe the high-energy electron impact scattering, is important for the normalization and understanding of the electron differential cross sections, particularly at small scattering angles, for obtaining integral cross sections, and optical oscillator strengths (OOS's), among other things. It has also been used to probe the intricate nature of the valence- and inner-shell electronic excitations, as well as to provide information about the nature of the electronic transitions and of the electron scattering process itself. The importance of the GOS in the study of electron-impact phenomena has been reviewed by Inokuti [2].

The use of angle-resolved electron energy-loss spectroscopy (EELS) to obtain absolute GOS measurements was pioneered by Lassette and co-workers [3]. They pointed out [4] that the GOS for a bound-state excitation can be expanded as an even power series of the momentum transfer (the so-called Lassette series). This technique has been widely used to obtain the electronic structure for many atoms, He, Ar, Ne, K, Xe, Hg, N, Li, Na, Kr [5–17], and molecules, CO, N<sub>2</sub>, NO, N<sub>2</sub>O, H<sub>2</sub>O, SF<sub>6</sub>, C<sub>2</sub>H<sub>2</sub>, CF<sub>3</sub>Cl, CF<sub>2</sub>Cl<sub>2</sub>, CFCl<sub>3</sub> [18–24], etc.

Theoretically, algebraic expressions were obtained by Shimamura [25] for the GOS of hydrogenlike atoms for the dipole allowed transitions with the principal quantum number  $n$  of 2, 3, and 4. Then, Ganas and Green [26] utilized the analytic atomic independent-particle model as a basis for calculating the GOS's for the single-particle excitations of Ne, Ar, Kr, and Xe. The average GOS's for the rare-gas atoms were also studied by Miller [27], employing hydrogenlike orbitals. Kim and Bagus [28] calculated GOS's for the lowest  $^1P$  transitions in Mg, Ca, Sr, and Ba using multiconfiguration Hartree-Fock wave functions. Their results substantially improved the Born cross sections. Davis and Sinanoglu [29] studied the influence of electron correlations on the GOS of open-shell transitions in neutral atoms Be, B, C, N, and O. However, their Hartree-Fock results are much higher than the experimental data. The second-order Born amplitude of the GOS in powers of the momentum transfer with a high-

energy exchange approximation was derived by Bonham and Goruganthu [30]. The GOS's for the argon  $3p$ - $4s$  and potassium  $4s$ - $4p$  transitions were also calculated, respectively, by Bielschowsky *et al.* [16] in Glauber approximation and by Mitroy [31] using a polarized potential in the scattering Hamiltonian.

Recently, Chen *et al.* [32] evaluated the minimum of the GOS for the oxygen  $2p^4(^3P) \rightarrow 2p^3(^4S)3s(^3S)$  transition. The calculated positions of the minima for the transitions in Ar, Ne, Kr, Xe, Na, and K, using the random-phase approximation with exchange (RPAE) and the spin-polarized technique of the RPAE (SPTRPAE) are some of the important results among the recent studies of the GOS [33–44]. These investigations have greatly enhanced the understanding of the GOS in these atoms.

The aim of this paper is to go beyond the previous studies of the GOS cited above and investigate the GOS's for inner-shell electron transitions. Toward this end, we derive a formula to evaluate the GOS for the transition  $|l^{n_1}, l^{n_2}\rangle \rightarrow |l^{n_1-1}, l^{n_2+1}\rangle$  and check it against the existing formula for the transition  $|l^{n_1}\rangle \rightarrow |l^{n_1-1}l'\rangle$ . We then illustrate the utility of the present formula by calculating the GOS for the sodium  $2p^63s(^2S) \rightarrow 2p^53s^2(^2P)$  transition and compare the results with the experimental data [39]. We also calculate GOS's for the carbon  $2s^22p^2(^3P) \rightarrow 2s2p^3(^3P)$  and  $2s^22p^2(^3P) \rightarrow 2s2p^3(^3D)$  transitions. The multiplet oscillator strengths evaluated using the present formula agree very well with the experimental data.

### II. THEORY

One advantage of the second-quantization formalism compared with coordinate representation is the ease of finding the expressions for the matrix elements of the complex electronic configurations. For the present purpose we use the expression of the GOS, in atomic units, given in [32]

$$f(q, w) = \frac{4w}{gq^2} \sum_k |T_k|^2, \quad (1)$$

where  $w$  is the excitation energy,  $q$  is the momentum transfer to the atom, and  $g$  is the statistical weight of the lower term

[45]. The reduced matrix element  $T_k$  is given by

$$T_k = (-1)^{L'} \sqrt{2\pi} i^k \langle L' S' || O^k || L S \rangle, \quad (2)$$

where  $L$ ,  $S$  and  $L'$ ,  $S'$  are, respectively, the total orbital angular momentum and spin of the initial and final state of the atom. The operator  $O^k$  acting only on orbital angular momenta is given by the second quantization in the coupled (tensorial) form [46],

$$O^k = \sqrt{\frac{[S]}{[k]}} \langle l' || Y_{kj_k}(qr) || l \rangle [a_{n'l'}^\dagger \times \tilde{a}_{nl}]^{(k0)}, \quad (3)$$

where

$$\begin{aligned} \langle l' || Y_{kj_k}(qr) || l \rangle &= (-1)^{l'} \sqrt{\frac{[l, l', k]}{(4\pi)}} \\ &\times \begin{pmatrix} l' & k & l \\ 0 & 0 & 0 \end{pmatrix} \int_0^\infty R_{n'l'} j_k(qr) R_{nl} r^2 dr. \end{aligned} \quad (4)$$

$[s]^{1/2} = \sqrt{2s+1}$ ,  $s$  is the spin of electron. Of course we always have  $s = \frac{1}{2}$ , but it seems best to retain the symbol  $s$  to bring out the similarity between the orbital and spin spaces. The operator  $a_{n'l'}^\dagger$  is the electron creation operator which is an

irreducible tensor operator of rank  $l'$  with respect to orbital angular momentum and of rank  $\frac{1}{2}$  with respect to the spin angular momentum. The electron annihilation operator, the Hermitian conjugate of the creation operator, is no longer the component of the irreducible tensor. Such a tensor is formed from  $(2l+1)(2s+1)$  components of the operator  $\tilde{a}_{lsm\nu} = (-1)^{l+s-m-\nu} a_{l's-m-\nu}$ .  $m$  and  $\nu$  are, respectively, the electron quantum numbers of the orbital angular momentum and spin in the  $z$  axis. The coupled double tensor  $[a_{n'l'}^\dagger \times \tilde{a}_{nl}]^{(k0)}$  can be uncoupled by using Eq. (34) of Ref. [47],

$$\begin{aligned} &\langle L' S' || [a_{n'l'}^\dagger \times \tilde{a}_{nl}]^{(k0)} || L S \rangle \\ &= \sqrt{\frac{[k]}{[S]}} (-1)^{S+S'+L+L'+k} \sum_{\bar{L}\bar{S}} \\ &\times \begin{Bmatrix} s & 0 & s \\ s' & \bar{s} & s \end{Bmatrix} \begin{Bmatrix} l & k & l' \\ L' & \bar{L} & L \end{Bmatrix} \\ &\times \langle L' S' || a_{n'l'}^\dagger || \bar{L}\bar{S} \rangle \langle \bar{L}\bar{S} || \tilde{a}_{nl} || L S \rangle. \end{aligned} \quad (5)$$

Since we have  $S=S'$ ,  $M_S=M'_S$  ( $M_S$  is the  $z$  component of the  $S$ ) and  $\Sigma M'_S=1$  a factor  $[S]^{-1/2}$  has to be added in the above equation. Performing the tensor algebra [48] of the operators  $a_{n'l'}^\dagger$  and  $\tilde{a}_{nl}$  we obtain

$$\begin{aligned} \langle L' S' || a_{n'l'}^\dagger || \bar{L}\bar{S} \rangle \langle \bar{L}\bar{S} || \tilde{a}_{nl} || L S \rangle &= \langle l^{n_1-1} [L'_1 S'_1] l'^{(n_2+1)} [L'_2 S'_2] L' S' || a_{n'l'}^\dagger || l^{n_1-1} [L'_1 S'_1] l'^{n_2} [L_2 S_2] \bar{L}\bar{S} \rangle \times \langle l^{n_1-1} [L'_1 S'_1] l'^{n_2} [L_2 S_2] \bar{L}\bar{S} || \tilde{a}_{nl} || \\ &\times |l^{n_1} [L_1 S_1] l'^{n_2} [L_2 S_2] L S \rangle \\ &= G_{L'_1 S'_1}^{L_1 S_1} G_{L'_2 S'_2}^{L_2 S_2} (-1)^{(n_1-1)+L'_1+L_2+L'+l'+S'_1+S_2+S'+s} [L', \bar{L}, S', \bar{S}]^{1/2} \begin{Bmatrix} L'_2 & L' & L'_1 \\ \bar{L} & L_2 & l' \end{Bmatrix} \begin{Bmatrix} S'_2 & S' & S'_1 \\ \bar{S} & S_2 & s \end{Bmatrix} \\ &\times (-1)^{n_2+1} \sqrt{n_2+1} [L'_2, S'_2]^{1/2} \times (-1)^{L'_1+L_2+L+l+S'_1+S_2+S'+s} [\bar{L}, L, \bar{S}, S]^{1/2} \begin{Bmatrix} L'_1 & \bar{L} & L_2 \\ L & L_1 & l \end{Bmatrix} \begin{Bmatrix} S'_1 & \bar{S} & S_2 \\ S & S_1 & s \end{Bmatrix} \\ &\times (-1)^{n_1} \sqrt{n_1} [L_1, S_1]^{1/2} (-1)^{L_1+S_1-l-s-L'_1-S'_1}, \end{aligned} \quad (6)$$

where  $G_{L'_1 S'_1}^{L_1 S_1} = (l^{n_1-1} [L'_1 S'_1]) \{ l^{n_1} [L_1 S_1] \}$  and  $G_{L'_2 S'_2}^{L_2 S_2} = (l'^{n_2} [L'_2 S'_2]) \{ l'^{(n_2+1)} [L_2 S_2] \}$  are the coefficients of fractional parentage. Substituting Eqs. (3)–(6) into Eq. (2) and noting the relationships,

$$\begin{Bmatrix} L_2 & L & L_1 \\ l' & k & l \\ L'_2 & L' & L'_1 \end{Bmatrix} = \sum_{\bar{L}} (-1)^{2\bar{L}} [\bar{L}] \begin{Bmatrix} L'_1 & \bar{L} & L_2 \\ L & L_1 & l \end{Bmatrix} \begin{Bmatrix} L' & k & L \\ l & \bar{L} & l' \end{Bmatrix} \begin{Bmatrix} L'_2 & L' & L'_1 \\ \bar{L} & L_2 & l' \end{Bmatrix}, \quad (7)$$

and

$$\sum_{\bar{S}} (-1)^{\bar{S}+S_1+S'_2} [\bar{S}] \begin{Bmatrix} S'_2 & S' & S'_1 \\ \bar{S} & S_2 & s \end{Bmatrix} \begin{Bmatrix} S'_1 & \bar{S} & S_2 \\ S & S_1 & s \end{Bmatrix} = \begin{Bmatrix} S'_1 & s & S_1 \\ S_2 & S & S'_2 \end{Bmatrix}. \quad (8)$$

Finally the matrix element  $T_k$  can be evaluated with

$$\begin{aligned}
T_k &= i^k \sqrt{\frac{n_1(n_2+1)}{2}} G_{L_1 S_1}^{L_1 S_1} G_{L_2 S_2}^{L_2 S_2} [S_1, S_2, L_2, L', L, L_1, l', l, k]^{1/2} \\
&\times (-1)^{S+S_2+S_1+l+L_2+L+L_2'+l'+n_2} \begin{Bmatrix} l' & k & l \\ L_2 & L & L_1 \\ L_2' & L' & L_1' \end{Bmatrix} \begin{Bmatrix} S_1' & s & S_1 \\ S_2 & S & S_2' \end{Bmatrix} \\
&\times \begin{pmatrix} l' & k & l \\ 0 & 0 & 0 \end{pmatrix} \int_0^\infty R_{n'l'j_k}(qr) R_{nl} r^2 dr. \quad (9)
\end{aligned}$$

Equation (9) represents a general formula to evaluate the GOS for the inner-shell transition between two open shells of atoms.

### III. RESULTS

Previously, the formula for the GOS of open-shell atoms was given, viz. for an electron transition of the form  $|l^{n_1}\rangle \rightarrow |l^{n_1-1}l'\rangle$ . By comparing the result in Ref. [32] with the current Eq. (9), we understand that Eq. (9) must reduce to the former result if we set  $n_2=0$  in Eq. (9).

We note that  $L_1=L$ ,  $L_2=0$ ,  $L_2'=l'$ ,  $S_2=0$ ,  $S_1=S$ ,  $S_2'=s$  when  $n_2=0$ , and the  $9j$  symbol is reduced to the  $6j$ -symbol,

$$\begin{pmatrix} l' & k & l \\ 0 & L & L \\ l' & L' & L_1' \end{pmatrix} = \frac{(-1)^{k+L_1'+L+l'}}{[L, L']^{1/2}} \begin{Bmatrix} L' & k & L \\ l & L_1' & l' \end{Bmatrix}, \quad (10)$$

and the  $6j$  symbol reduces to

$$\begin{Bmatrix} S_1' & s & S \\ 0 & S & s \end{Bmatrix} [S, s]^{1/2} (-1)^{2(S_1'+s+S)} = 1. \quad (11)$$

Substituting Eqs. (10) and (11) into Eq. (9), the matrix element  $T_k$  becomes

$$\begin{aligned}
T_k &= i^k \sqrt{\frac{n_1}{2}} G_{S_1' L_1'}^{S L} (-1)^{k+L_1'+l+l'} [L', L, l', l, k]^{1/2} \\
&\times \begin{pmatrix} L' & k & L \\ l & L_1' & l' \end{pmatrix} \begin{pmatrix} l' & k & l \\ 0 & 0 & 0 \end{pmatrix} \int_0^\infty R_{n'l'j_k}(qr) R_{nl} r^2 dr. \quad (12)
\end{aligned}$$

Equation (12) will give the same GOS value as Eqs. (6) and (7) of Ref. [32], except that the latter has a mistake in  $[L, L']$ . The correct one is  $[L, L']^{1/2}$ .

The sodium  $2p$ - $3s$  transition is a special situation of the inner-shell transition. The initial subshell is a closed shell while the final subshell is also a closed shell. In that case we have  $G_{S_1' L_1'}^{S_1 L_1} = 1$ ,  $G_{S_2' L_2'}^{S_2 L_2} = 1$ ,  $L_1=0$ ,  $L_2=0$ ,  $l=1$ ,  $L=0$ ,  $L_1'=1$ ,  $L_2'=0$ ,  $l'=0$ ,  $L'=1$ ,  $n_2=1$ . Substituting these parameters into Eqs. (9) and (1), we have

$$\begin{aligned}
f(q, w) &= \frac{2w}{gq^2} \sum_k [k] [l', l]^{1/2} \begin{pmatrix} l' & k & l \\ 0 & 0 & 0 \end{pmatrix} \\
&\times \int_0^\infty R_{n'l'j_k}(qr) R_{nl} r^2 dr. \quad (13)
\end{aligned}$$

When  $g=1$  Eq. (13) represents the expression for a closed-

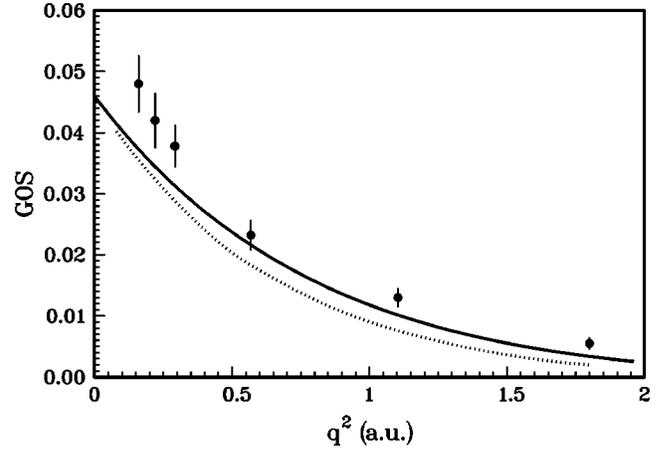


FIG. 1. GOS's vs  $q^2$  for sodium  $2p^6 3s(2S) \rightarrow 2p^5(2P) 3s^2(2P)$  transition. The solid line is the present results using the spin polarized technique of the random-phase approximation with exchange. The dotted line represents the Hartree-Fock calculation and the small black dots are from the measurement of Bielschowsky *et al.* [39].

shell atom. Therefore  $gf(q, w)$  for the sodium  $2p$ - $3s$  transition can be calculated with the closed-shell expression Eq. (13). This equation has been used in Ref. [39]. The fact that Eq. (9) reduces to the closed-shell formula for the Na  $2p$ - $3s$  transition is another powerful check of Eq. (9).

In the present calculation, the radial part of the wave functions for each state was represented by 700 points. The SPTRPAE was also used in the calculation to include the correlation among the subshells  $p$ - $s$ ,  $p$ - $d$ , and  $s$ - $p$ . The present GOS results are plotted with the experimental data in Fig. 1. The dotted and solid curves are, respectively, the Hartree-Fock and the SPTRPAE results. The black dots are the experimental data [39]. As we stated before, the present Hartree-Fock results are the same as those in Ref. [39]. The calculated results including correlation effects (solid curve) are closer to the experimental data, indicating the importance of correlations for this sodium transition. However, from the well-known behavior of the GOS in the limit  $q^2 \rightarrow 0$ , it appears that the experimental data rise more rapidly in comparison with the calculated results. Unfortunately, the OOS for this sodium transition is not available. There is a great need for an independent value of the OOS to check both the measurement and the present calculation. Suffice to state that the present general formula Eq. (9) for the GOS indeed reduces to that of Ref. [32] and is applicable to inner-shell transitions between two open shells of atoms.

Figures 2 and 3 represent the GOS's versus  $q^2$  calculated in Hartree-Fock wave functions for the carbon  $2s^2 2p^2(3P) \rightarrow 2s 2p^4(3P)$  and  $2s^2 2p^2(3P) \rightarrow 2s 2p^4(3D)$  transitions, respectively. The solid and the dash-dot curves are the present results in the velocity and the length forms, respectively. When  $q^2 \rightarrow 0$ , the GOS converges to the optical oscillator strength. In the present case the GOS should approach the multiplet oscillator strength as  $q^2 \rightarrow 0$ .

The multiplet oscillator strengths from the present calculation are 0.0659 (length) and 0.0610 (velocity) for the carbon  $2s^2 2p^2(3P) \rightarrow 2s 2p^4(3P)$  transition, which agree excel-

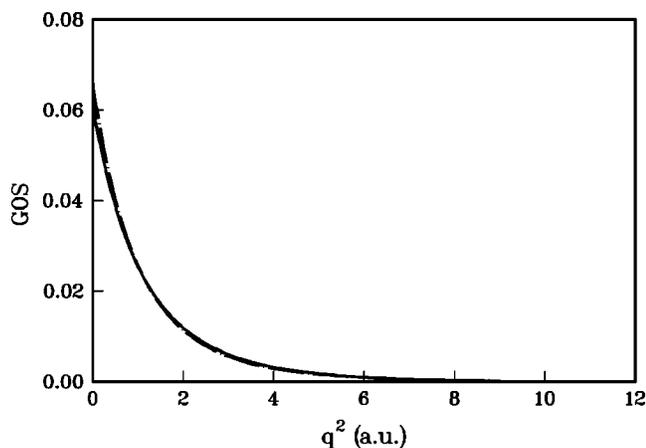


FIG. 2. GOS's versus  $q^2$  for carbon  $2s^2 2p^2(^3P) \rightarrow 2s 2p^3(^3P)$  transition. The solid and dash-dot curves are the present results in velocity and length forms, respectively.

lently with the experimental result of 0.0634 [49]. The multiplet oscillator strengths for the carbon  $2s^2 2p^2(^3P) \rightarrow 2s 2p^3(^3D)$  transition from the present calculations are 0.0953 (length) and 0.114 (velocity), which are in reasonable agreement with the value of 0.0718 given in Ref. [49]. Davis and Sinanoglu [29] also calculated the GOS for the same reactions. Their multiplet oscillator strengths computed using Hartree-Fock wave functions approach the values of 0.202 and 0.286, which are several times larger than the 0.0634 and 0.0718 of Ref. [49], respectively. It is true that the total spin of the system and the projection of the spin will not change during the collision since the operator  $\sum_i^n \exp(i\mathbf{q} \cdot \mathbf{r}_i)$  is not a function of the spin. However, this should not cancel the factor of  $1/(2S_0+1)$ . This may be one of the reasons why their [29] Hartree-Fock results are much higher than those in Ref. [49].

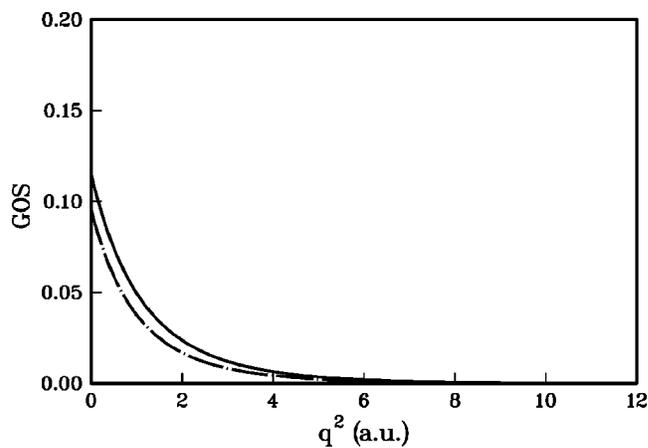


FIG. 3. GOS's versus  $q^2$  for carbon  $2s^2 2p^2(^3P) \rightarrow 2s 2p^3(^3D)$  transition. The curves have the same meaning as those in Fig. 2.

#### IV. CONCLUSION

A second-quantization formalism has been used to derive a general formula to calculate the GOS's for the inner-shell electron transitions between two open-shells of an atom. Equation (9) has been checked against previous results [32] and used to evaluate the GOS of the sodium  $2p^6 3s(^2S) \rightarrow 2p^5 3s(^2P)$  transition in the Hartree-Fock approximation and the random-phase approximation with exchange. The GOS for the carbon  $2s^2 2p^2(^3P) \rightarrow 2s 2p^3(^3P)$  and  $2s^2 2p^2(^3P) \rightarrow 2s 2p^3(^3D)$  transitions have also been evaluated. The multiplet oscillator strengths obtained with the present formula are found to be in good agreement with the values in Ref. [49].

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