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Minima in generalized oscillator strengths of atomic transitions and the approach to the high-energy limit

N. B. Avdonina,[1,4] D. Fursa,[2] A. Z. Msezane,[3] and R. H. Pratt[4]
[1]*Department of Electrical Engineering, University of Alaska Fairbanks, Fairbanks, Alaska 99770, USA*
[2]*School of Engineering Science, Murdoch University, Perth, Western Australia 6150, Australia*
[3]*Department of Physics & Center for Theoretical Studies of Physical Systems, Clark Atlanta University, Atlanta, Georgia 30314, USA*
[4]*Department of Physics and Astronomy, University of Pittsburgh, Pittsburgh, Pennsylvania 15260, USA*
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Minima in the generalized oscillator strength (GOS) and the convergence of the GOS to the first Born approximation (FBA) limit for the Ba $6s\ ^1S \rightarrow 6p\ ^1P$ optically allowed transition are investigated. The random-phase approximation with exchange, which takes into account correlation effects among the atomic electrons themselves, and the convergent close-coupling (CCC) approximation are used for the calculations. We find the following. (1) The GOS as a function of the momentum transfer squared K^2 is characterized by a complex structure of multiple minima, significantly different in the two approximations and approaches the high-energy FBA limit only at small K^2 values (less than about 0.5 a.u.). (2) The number of minima calculated in the CCC approximation increases with increase in energy, but does not correspond to the number obtained in the FBA, even at high energy $\sim$1 keV. The CCC and FBA minima are in general not directly related. The FBA minima, except for the first, do not correspond to physical observables at these energies. (3) At high energy the interaction between the incident electron and the target remains significant, resulting in slowing down the convergence of the CCC GOS to the corresponding nonrelativistic FBA results.

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I. INTRODUCTION

The generalized oscillator strength (GOS), introduced by Bethe [1] and discussed further by Inokuti [2], provides information on both the valence and inner-shell excitations of atoms and molecules and is important in radiation physics, plasma research, astrophysics, and laser development. The GOS, as a function of the momentum transfer squared K^2, is characterized by a complex structure of minima, which are essentially a manifestation of the properties of the radial parts of the initial- and final-state wave functions. Recent experimental and theoretical investigations have revealed that the minima characterize the GOS of the noble-gas and alkali-metal atoms in the region $K^2 \rightarrow 0$. These minima may create problems in the extrapolation of the GOS function to the optical limit ($K=0$) in the determination of precise dipole oscillator strengths. The theoretical investigations have concentrated mainly on the precise location of the positions of the minima and their sensitivity to electron correlation effects in the atom. In this paper we also investigate the sensitivity to effects beyond a plane-wave description of the projectile electron, and we examine how the positions and number of the minima change as the incident energy E increases.

Due to its simplicity, the nonrelativistic first Born approximation (FBA), which omits distorted-wave effects and correlations between the projectile and atomic electrons, but assumes some particular description of the target, is often used for the calculation of GOS's at high incident electron energy. The use of the FBA is encouraged by the theorem [3] which states that the nonrelativistic GOS's for inelastic electron-atom scattering, for any fixed value of K approach the FBA result in the high-energy limit (assuming the same description of the target is used for the calculation of GOS's in the FBA). The goal of this paper is to investigate how the positions of the GOS minima [calculated here in the convergent close-coupling (CCC) approximation] approach the positions of the minima calculated in the nonrelativistic FBA as the incident energy increases. The main question is how rapidly the FBA limit is approached, since with increase of the incident energy relativistic effects begin to play a significant role.

Previously the random-phase approximation with exchange (RPAE) [4] calculations, which take into account correlation effects among the atomic electrons and used within the framework of the FBA ($\mathrm{RPAE_{BA}}$), investigated the precise location of the lowest minima [5–10]. For the noble gases Ne, Kr, and Xe [5] the positions of the minima were found to be insensitive to exchange and correlation effects among the atomic electrons, and the $\mathrm{RPAE_{BA}}$ calculations agreed excellently with measurements [11–13] on their locations. The measurements were carried out at electron impact energies of 2.5 keV [11] and down to even smaller energies (500 and 300 eV) [12,13]. Recently, absolute GOS's for the excitation of Kr to the $5s$ and $5p$ levels over a wide K^2 region at 2.5 keV impact energy have been measured [14]. While excellent agreement between the measurement and the $\mathrm{RPAE_{BA}}$ calculation [5] has been obtained for the position of the minimum, there are significant differences among the various measurements [11,13,14], which have been discussed [14] (these include the normalization of the relative measurements, influence of angular resolution, and pressure effects). The $\mathrm{RPAE_{BA}}$ GOS results for the Ar $3p \rightarrow 4s$ transition were compared with those measured by Fan and Leung [15], Li *et al.* [16], and Bielschowsky *et al.* [17]. The calculated position [10] of the lowest minimum agreed excellently with

the measured one. It was noticed, however, that calculations based on the FBA appear to be in reasonable agreement with the measured GOS data at 2.5 keV only in shape, and also for $K^2<1$ a.u., while for higher K values the Glauber approximation works much better [14].

GOS's for the resonance transitions in Mg and Na were calculated in [6,8]. Unlike the noble gases, the correlations were found to influence the positions of the minima significantly, particularly in Mg. However, while there is agreement [18] on the position of the first minimum in Mg, experimental determinations of its position in Na vary significantly [19–22]. For the potassium $4s\rightarrow 4p$ transition $\mathrm{RPAE_{BA}}$ calculations [7] found two minima at low K values, one narrower and not observed and the other at a higher value of K, confirmed experimentally [23–25], but whose position is sensitive to the atomic electron correlations.

To investigate minima in the GOS and the convergence of the GOS to the FBA limit three calculations have been performed for the Ba $6s\ ^1S\rightarrow 6p\ ^1P$ transition: (1) the $\mathrm{RPAE_{BA}}$, where we have used plane waves for the initial and final electronic wave functions; (2) the CCC approximation [26], which includes both distorted-wave effects and correlations between the projectile and target electrons in the energy range below 1 keV; and (3) the FBA with Hartree-Fock (HF) target wave functions ($\mathrm{HF_{BA}}$) as well as with configuration-interaction (CI) wave functions ($\mathrm{CI_{BA}}$). The CCC approach, at energies where it can be used, is probably one of the most accurate approaches available, and it generally gives results in good agreement with experiments.

For the $6s\ ^1S\rightarrow 6p\ ^1P$ transition in Ba we investigate both the magnitude of the GOS's, and the positions and character of the minima. Our choice of Ba is dictated by several factors. (1) We noted that in all $\mathrm{CI_{BA}}$, $\mathrm{HF_{BA}}$, and $\mathrm{RPAE_{BA}}$ results the GOS's for Ba have a complex structure, dominated by minima, and the first minimum occurs at relatively low K values. (2) For the $6s\ ^1S\rightarrow 6p\ ^1P$ transition in Ba these minima of the GOS's calculated in the $\mathrm{RPAE_{BA}}$ are very sharp, reaching zero, so that it is easier to see the energy dependence of the non-Born terms which fill in the zeros, resulting in nonzero minima (the positions of the minima also change when we go beyond the corresponding FBA). (3) For our calculations it was important that, since Ba has a filled s subshell, GOS's for the $6s\ ^1S\rightarrow 6p\ ^1P$ transition in Ba could be easily and accurately calculated in both $\mathrm{HF_{BA}}$ and $\mathrm{RPAE_{BA}}$ approaches. We can also perform calculations in the CCC approximation [26], which has been shown to be accurate for electron scattering from atoms with two valence electrons [27,28], and compare results with those from $\mathrm{CI_{BA}}$ calculations.

We started our CCC calculations at incident energies close to threshold and found that the GOS's have a structure which is characterized by multiple extrema in the whole region of allowed K values, even at low $E=5$ eV. With increasing E the magnitude (away from the minima) of the GOS's decreases, but even at the highest E (about 900 eV), for which we could calculate in the CCC approximation, the magnitude is still much higher than predicted by $\mathrm{CI_{BA}}$. Only the first minimum, at small K tends, with increasing incident energy, to the position (independent of energy) of the first zero of the $\mathrm{CI_{BA}}$ matrix element. We have not found any convergence to the $\mathrm{CI_{BA}}$ result for the region of K values beyond that of the first minimum, up to $E\cong 900$ eV. Additional minima in the CCC results appear with increasing energy at higher values of K throughout the range of energies up to $E\cong 900$ eV, but neither their number nor their positions correspond to those obtained in the $\mathrm{CI_{BA}}$ approach.

TABLE I. Acronyms and variables used in the paper.

CCC	Convergent close-coupling
FBA	First Born approximation
CI	Configuration interaction
HF	Hartree-Fock
RPAE	Random-phase approximation with exchange
$\mathrm{CI_{BA}}$	First Born approximation used with CI wave functions
$\mathrm{HF_{BA}}$	First Born approximation used with HF wave functions
$\mathrm{RPAE_{BA}}$	Random-phase approximation with exchange used with plane waves for the initial and final electron wave functions
GOS; $f_\omega\ (E,K)$	Generalized oscillator strength; GOS function
OOS; f_ω	Optical oscillator strength; OOS function
K	Momentum transfer
E	Electron impact energy
ω	Energy transfer

For convenience we have created a table of abbreviations given by Table I.

II. MINIMA OF GENERALIZED OSCILLATOR STRENGTHS IN THE $6s\ ^1S\rightarrow 6p\ ^1P$ TRANSITION IN BARIUM

The GOS for excitation is defined in terms of the incident energy E, energy transfer ω, and momentum transfer K [1] as (atomic units are used throughout).

$$f_\omega(E,K)=\frac{\omega}{2}\frac{p_i}{p_f}K^2\sigma, \tag{1}$$

where $p_{i,f}$ are the electron momenta before and after the collision, respectively, and σ is the measured or calculated differential cross section $\sigma=d\sigma/d\Omega$. The momentum transfer depends on E, ω, and the scattering angle θ through

$$K^2=2E\left[2-\frac{\omega}{E}-2\sqrt{\left(1-\frac{\omega}{E}\right)}\cos\theta\right]. \tag{2}$$

The differential cross section σ in Eq. (1) is obtained by averaging the square of the scattering amplitude A_{m_i,m_f} over the magnetic sublevels m_i of the initial-state orbital angular momentum ℓ_i and summing it over the magnetic sublevels m_f of the final-state orbital angular momentum ℓ_f, so that

$$\frac{d\sigma}{d\Omega} = \frac{N_{\ell_i}}{2\ell_i + 1} \sum_{m_i m_f} |A_{m_i,m_f}|^2, \tag{3}$$

where N_{ℓ_i} is the number of electrons in the initial state. In the LS coupling scheme the amplitude A_{m_i,m_f} can be written in the form [29]

$$A_{m_i,m_f} = i^L \frac{4\sqrt{\pi}}{K^2} \sqrt{\frac{k_f}{k_i}} \sqrt{\frac{2\ell_f + 1}{2\ell_i + 1}} \sum_{L=|\ell_i-\ell_f|}^{\ell_i+\ell_f} (2L + 1) C^{\ell_i 0}_{\ell_f 0 L 0} C^{\ell_i m_i}_{\ell_f m_f L(m_i-m_f)} M^L_{fi} Y_{L(m_i-m_f)}(\theta_K), \tag{4}$$

where the Clebsch-Gordan coefficients $C^{\ell_i m_i}_{\ell_f m_f L(m_i-m_f)}$ and the spherical harmonics $Y_{L(m_i-m_f)}(\theta_K)$ are defined according to [30]. The angle θ_K is related to the scattering angle θ through $\cos\theta_K = (k_i - k_f \cos\theta)/K$.

For transitions from an initial ^1S ground state, as in Ba, the summation over $m_{i,f}$ in Eq. (3) reduces to summation only over m_f, with $m_i = 0$, and in the case of an optically allowed transition, such as the $6s\ ^1S \rightarrow 6p\ ^1P$ of Ba, the summation over L in Eq. (4) reduces to the one term $L = 1$. Substitution of plane waves for the wave functions of the initial and scattered electrons in the matrix element M^L_{fi} of Eq. (4) makes the expression for A_{m_i,m_f} even simpler, reducing the summation over m_f in Eq. (3) to one term. We then have

$$M_{s\rightarrow p}(\omega, K) = -6 \int_0^\infty R_1(r) j_1(Kr) R_0(r) r^2 dr. \tag{5}$$

Here $R_{0,1}$ are the initial and final one-electron radial wave functions of the active atomic electron, respectively, and $j_1(Kr)$ is the spherical Bessel function.

The matrix element of Eq. (5) with $R_{0,1}$ calculated in the $\mathrm{HF_{BA}}$ approximation, $M^{\mathrm{HF}}_{s\rightarrow p}$ is used as a zero-order approximation to include the atomic target electron correlations. In the $\mathrm{RPAE_{BA}}$ $M^{\mathrm{RPAE}}_{s\rightarrow p}$ is a solution of the equation [31,32]

$$M^{\mathrm{RPAE}}_{s\rightarrow p}(\omega, K) = M^{\mathrm{HF}}_{s\rightarrow p}(\omega, K) + \left(\sum_{(n<F)} \int - \sum_{(\varepsilon>F)} \int \right) \times \frac{M^{\mathrm{RPAE}}_{s\rightarrow p}(\omega, K) \langle ns|U|\varepsilon p\rangle}{\omega - \omega_{sp} \pm i\delta}, \tag{6}$$

where $\langle n|$ represents all possible vacancies for the atomic electrons, and $|\varepsilon\rangle$ represents all possible virtual excited states, F is the Fermi energy, and the infinitesimally small quantity $i\delta$ has a + sign for the first summation and a − sign for the second one. Note that for the excitations to the discrete levels $6s \rightarrow np$ the difference in energies of the $6s$ and np states, $\omega_{sp} = E_p - E_s$, is altered due to the influence of residual interactions [4], and $M^{\mathrm{RPEA}}_{s\rightarrow p}(\omega, K)$ does not have a pole at $\omega = \omega_{sp}$. As a consequence, $M^{\mathrm{RPAE}}_{s\rightarrow p}$ is real (not complex), just as is $M^{\mathrm{HF}}_{s\rightarrow p}(\omega, K)$ in Eq. (5).

According to [33], for neutral atoms the $f_\omega(E,K)$ in Eq. (1) for optically allowed transitions behaves as $\lim_{K^2\rightarrow 0} f_\omega(E,K) = f_\omega$ for any impact energy E, where f_ω is the optical oscillator strength. Thus, generally, at least for high-energy scattering, $f_\omega(E,K)$ is a monotonically decreasing function of K, starting from a pronounced maximum in the forward scattering direction or nearby. With increasing scattering angle the difference in the periods of oscillations of the initial and final wave functions of the projectile electron increases, and that decreases the partial matrix elements M^L_{fi} of the process. Consequently, $f_\omega(E,K)$ decreases as K increases.

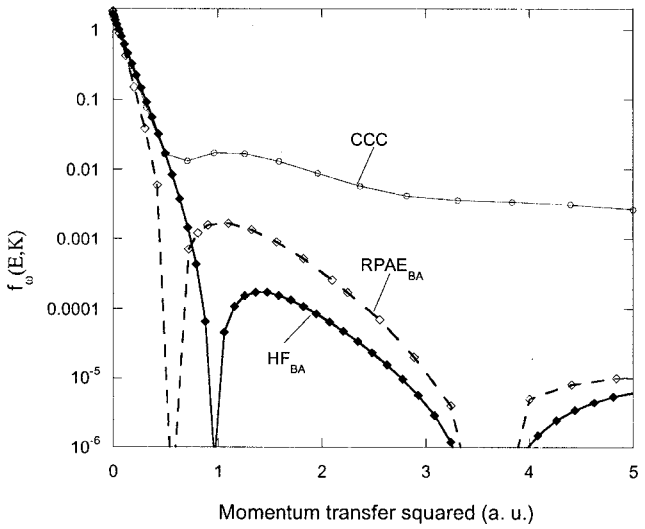

FIG. 1. Comparison of the GOS for the Ba $6s\ ^1S \rightarrow 6p\ ^1P$ excitation in the vicinity of the first two minima. The $f_\omega(E,K)$ are calculated in the $\mathrm{HF_{BA}}$, $\mathrm{RPAE_{BA}}$, and CCC approximations at $E = 897.5$ eV.

It can happen, however, that the real matrix elements $M^{\mathrm{HF}}_{s\rightarrow p}$ and $M^{\mathrm{RPAE}}_{s\rightarrow p}$ for the discrete excitations, as functions of K, change sign while decreasing, so that the $f_\omega(E,K)$ has a zero. That can result in a minimum in the total $f_\omega(E,K)$ in its dependence on K [2]. Generally, the radial matrix element M^L_{fi} in Eq. (4) is complex. Consequently, and also due to the summation in Eq. (3), $f_\omega(E,K)$ will generally have nonzero minima, in contrast to the minima of the $f_\omega(E,K)$ calculated in the $\mathrm{HF_{BA}}$ or $\mathrm{CI_{BA}}$ approximation, or for the excitations in the $\mathrm{RPAE_{BA}}$. Note that for small K values the reason for a minimum in $f_\omega(E,K)$ can be similar to the reason for a minimum in f_ω, the well-known Cooper minima [34] for transitions in photoprocesses [35]. Since the $f_\omega(E,K)$ reaches f_ω at $K = 0$ [33], the existence of a Cooper minimum leads to a minimum in the $f_\omega(E,K)$, considered as a function of ω. However, there can be other $f_\omega(E,K)$ minima, which are not associated with f_ω minima.

In Fig. 1 we show GOS functions $f_\omega(E,K)$ for the $6s\ ^1S \rightarrow 6p\ ^1P$ transition in Ba as a function of K^2. The first minima of the Ba $6s\ ^1S \rightarrow 6p\ ^1P$ excitation in the $\mathrm{RPAE_{BA}}$ and $\mathrm{HF_{BA}}$ are close to each other, and as seen in Fig. 1, the second $\mathrm{HF_{BA}}$ minimum nearly coincides with the second minimum in the $\mathrm{RPAE_{BA}}$, consistent with our statement about the decreasing difference between correlated and $\mathrm{HF_{BA}}$ results with increasing K. In Fig. 1 we also show $f_\omega(E,K)$ calculated in the CCC approximation (we give a description of this approximation in Sec. III) at $E = 897.5$ eV. The position of the first minimum in the CCC results is located between the $\mathrm{RPAE_{BA}}$ and $\mathrm{HF_{BA}}$ minima. Contrary to the zero-value minima obtained in the FBA, the first minimum in the

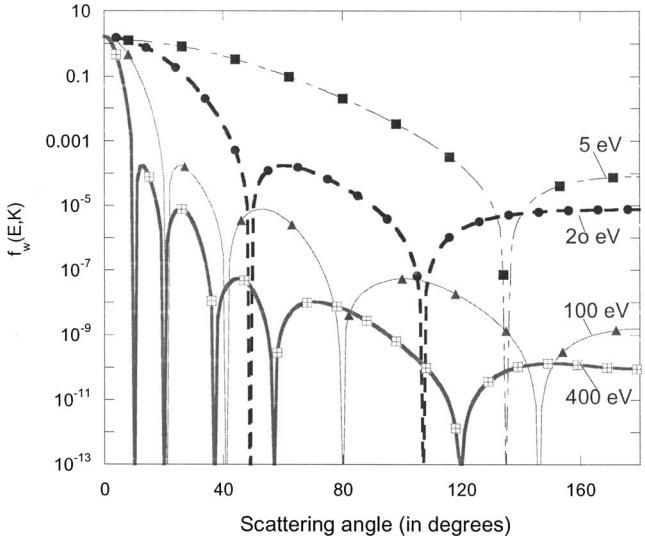

FIG. 2. GOS's for the Ba $6s\ ^1S \rightarrow 6p\ ^1P$ excitation, $f_\omega(E,K)$ calculated in the HF_{BA} method as functions of scattering angle θ at $E=5$, 20, 100, and 400 eV, where θ, E, and K are related through Eq. (2).

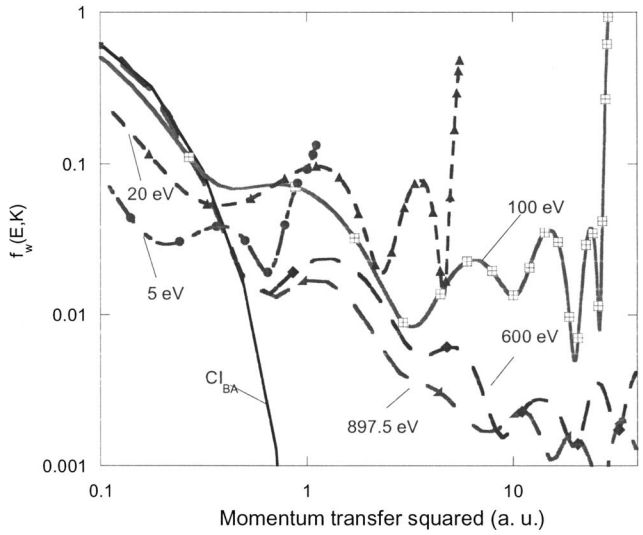

FIG. 3. GOS's $f_\omega(E,K)$ for the Ba $6s\ ^1S \rightarrow 6p\ ^1P$ excitation calculated in CI_{BA} and CCC approximations at $E=5$, 20, 100, 600, and 897.5 eV.

CCC approach is very shallow, while the second CCC minimum is nearly washed out.

Since the range of possible physical values of K becomes narrower with decreasing E, fewer minima are exposed in the physical region of the $f_\omega(E,K)$ curves. In Fig. 2 we show this effect for Ba $6s\ ^1S \rightarrow 6p\ ^1P$ excitation, for the HF_{BA} $f_\omega(E,K)$ as a function of the scattering angle θ for different values of E, rather than of K^2 as in Fig. 1. While at $E=400$ eV the HF_{BA} $f_\omega(E,K)$ has five minima, there is only one minimum at $E=5$ eV. Note that, although the HF_{BA} $f_\omega(E,K)$ depends only on K^2, independent of E, as a function of θ the $f_\omega(E,K)$ changes with energy consistent with the relation Eq. (2).

III. CONVERGENCE OF CCC TO CI_{BA} RESULTS

To analyze the importance of the interaction of the projectile electron with the Ba target, we have calculated $f_\omega(E,K)$ in the CCC approximation [26], which has been found to give the best agreement with experiment [36,37] for $6s\ ^1S \rightarrow 6p\ ^1P$ excitation in Ba [27]. The CCC GOS results for this transition were obtained previously [27]. The calculations were performed in the nonrelativistic LS coupling scheme using a configuration-interaction expansion. The target wave functions of the valence electrons were calculated in the frozen HF field of the Ba^+ ionic core together with a phenomenological core-polarization potential [38] added to fit the one-electron ionization energies of the Ba^+ ion. Another phenomenological two-electron polarization potential [39] was included in the total Hamiltonian of Ba in addition to the Coulombic electron-electron potential. Relativistic effects were found not to be important at the considered energies. More details of the CCC method can be found in [27,28]. The $f_\omega(E,K)$ calculated for the $6s\ ^1S \rightarrow 6p\ ^1P$ excitation in Ba in both the CCC approximation (for electron impact energies $E=5$, 20, 100, 600, and 897.5 eV) and in the corresponding CI_{BA} method are presented in Fig. 3. Here we have used the radial matrix elements M_{fi}^L [Eqs. (3) and (4)] calculated previously in [27].

Our choice of the target (barium), with its complex multiminima structure obtained in the CI_{BA} approach, allows us to observe the changes in $f_\omega(E,K)$ values and in the positions of extrema with increasing initial electron energy. It is seen (Fig. 3) that at small K^2 the 897.5 and 600 eV curves approach the CI_{BA} curve, while for all K^2 values greater than about 0.5 a.u., even at the very high energy of 897.5 eV, the CCC $f_\omega(E,K)$ are much larger than the CI_{BA} results. The lower-energy curves have much flatter behavior than the former curves, reaching the zero-angle curve (not the CI_{BA} curve) at small K and terminating there. The number of minima differs for the different energies E, being less for lower energies, because of the decreasing range of allowed K values. Note that the positions of the minima, as a function of K, obtained in the CCC approximation are only slightly correlated with those obtained in the CI_{BA} method, even at relatively small K^2 and high $E=897.5$ eV, where we can expect better applicability of CI_{BA} (Fig. 4). The CCC minima at this energy are very shallow, and we have not found convergence to the CI_{BA} results for the region of K values beyond the first minima; only the position of the first minimum converges to the CI_{BA} result.

Our results show that for high values of K a realistic result can be obtained by taking into account the interaction of the incident electron with the target. This interaction is very significant, slowing the convergence of the CCC $f_\omega(E,K)$ to the corresponding nonrelativistic Born result. Since distorted-wave approximations, both relativistic [40] and nonrelativistic [41], are in good agreement, in shape and absolute values, with experiment and with the CCC calculations [27] (at $E=60$ eV and above, up to 100 eV, considered in [40,41]), we can assume that distorted-wave approximation corrections are the most important in the convergence to the FBA.

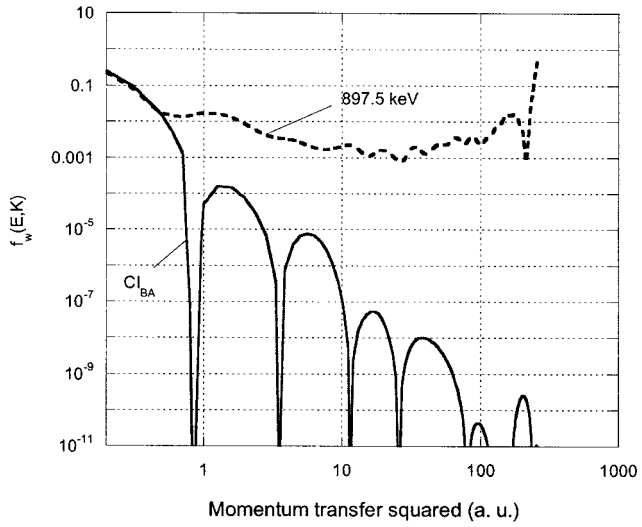

FIG. 4. Comparison of the GOS's for the Ba $6s\ ^1S \rightarrow 6p\ ^1P$ excitation at $E=897.5$ eV. The $f_\omega(E,K)$ are calculated in the CI_{BA} and CCC approximations.

To understand the reason for the slow convergence of the CCC to the CI_{BA} results we calculated the scattering amplitudes A_{m_i,m_f} for different values of E. In the CCC approximation the matrix elements are no longer real, and A_{m_i,m_f} is complex, due to the interaction of the scattered electron with electrons of the target. For the first two (lowest-K) minima we note that the imaginary part of A_{m_i,m_f} rapidly converges relative to the amplitude obtained in the CI_{BA} method with increase of E, but the real part of A_{m_i,m_f} is negligibly small only for small K^2 values. This explains why the $f_\omega(E,K)$ calculated in the CCC approximation are very close to the CI_{BA} results only for $K^2<0.5$ a.u.

With increase in K^2 the real part of the scattering amplitude plays a more and more important role, decreasing only slowly even at high values of E. For instance, in the vicinity of the first minimum it is already significant. This explains why the CCC calculations give only a shallow minimum in $f_\omega(E,K)$ at small K^2. Our calculations show that for large values of K^2 the real part of the scattering amplitude is of the same importance as the imaginary part, and we note that for such K^2 values the minima of $f_\omega(E,K)$ occur due to zeros in either the imaginary or real part of A_{m_i,m_f}, thus making the analysis more complicated.

IV. SUMMARY AND CONCLUSION

In this paper we have investigated the minima in GOS's for the $6s\ ^1S \rightarrow 6p\ ^1P$ excitation of Ba obtained from nonrelativistic CCC calculation for different energies of the incident electron and compared these results with those calculated in the corresponding CI_{BA}, $RPAE_{BA}$, and HF_{BA} methods. We have found that the GOS as a function of K^2 is characterized by a complex structure, dominated by multiple minima, whose number decreases with decreasing E. Howver, the number of minima in Ba $6s\ ^1S \rightarrow 6p\ ^1P$ calculated in the CCC approximation does not correspond to that obtained in the CI_{BA} method even at quite high incident energies. Furthermore, CI_{BA} calculations strongly disagree with the CCC results in the vicinity of the minima, even at high energy $\sim$1 keV. The positions of the CCC and FBA minima are in general not directly related. However, we do find that the position of the characteristic first minimum of the GOS, corresponding to small K^2 values, rapidly converges to the position obtained in the CI_{BA} method. Even at low energies it approximately corresponds to the zero of the Born matrix element. Clearly, it is the small K^2 values that determine the region of applicability of the CI_{BA} approach, and not necessarily the requirement of large E.

In our $RPAE_{BA}$ calculation for Ba the positions of the minima are shifted, relative to those of the HF_{BA} as well as those of the CI_{BA} calculation, especially at small K^2 values. This result demonstrates the importance of correlations due to the interactions of the atomic electrons at low K. However, the difference in behaviors of the GOS's calculated in all the above three ways is not as significant as the difference between them and the CCC results. The CCC approximation, which allows us to include distorted-wave effects as well as the correlation interaction between the incident electron and the atomic subshells, gives good agreement with experiment for the GOSs of Ba [36,37]. This reflects that the deviation of the wave functions of the incident and scattered electrons from plane waves plays a very important role at these energies.

We find that the convergence of the GOS for the $6s\ ^1S \rightarrow 6p\ ^1P$ excitation of Ba calculated in the CCC approximation to the nonrelativistic CI_{BA} high-energy limit is rather slow, just as was seen (for all atoms) for the optical oscillator strengths of the corresponding photoionization process [42,43]. The CI_{BA} predictions for the GOS are not realized in the first keV for excitation of the valence electron in Ba, and the FBA minima, except for the first, do not correspond to physical observables at these energies. Some slowly convergent factors, such as the Stobbe factor, which characterizes convergence in photoionization [42,43], associated with the Coulomb distortion of the plane waves, may be anticipated. We expect our results for Ba to be typical of many atomic transitions.

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