

Calculations of generalized oscillator strength for electron-impact excitations of krypton and xenon using a relativistic local-density potential

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The generalized oscillator strength (GOS) of an atom is an essential factor in the differential cross section for inelastic scattering of fast charged particles. Recently, Takayanagi *et al.* [Phys. Rev. A **41**, 5948 (1990)] have obtained the GOS for the excitation of atomic krypton to the $4p^5(^2P_{1/2})5s$ and $4p^5(^2P_{3/2})5s$ states from inelastic-scattering measurements using electron-energy-loss spectroscopy. The present study was undertaken with the twofold objective to determine the results of theoretical computations of the scattering parameters of the above experiment and to examine the suitability of a recently developed relativistic local-density-potential method [M. Vijayakumar, N. Vaidehi, and M. S. Gopinathan, Phys. Rev. A **40**, 6834 (1989)] to study atomic-collision processes. Calculations have been done to obtain GOS for electron-krypton and electron-xenon collisions in the squared-momentum-transfer range of 0.01 to 10 atomic units. The well-known theory of Bethe has been used for the determination of the GOS in the first-order Born approximation. The present results are in fair agreement with previous Hartree-Slater and Hartree-Fock calculations and with the experimental data available in the literature. Furthermore, results of the present calculations predict that the GOS goes through a minimum, similar to the "Cooper minimum" in the photoabsorption cross section, as a function of the value of the momentum transfer. Experiments at slightly higher values of momentum transfer are suggested to verify the position of this minimum.

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I. INTRODUCTION

Atomic-collision processes play an important role in the modeling of high-temperature plasmas, design of fusion reactors, and in pumping mechanisms in gas lasers. There is substantial recent interest in atomic-collision processes [1], and sophisticated experiments on inelastic scattering of electron beams are being conducted. Recently, Takayanagi *et al.* [2] have obtained the generalized oscillator strength (GOS) for excitation of atomic krypton to the $4p^5(^2P_{1/2})5s$ and $4p^5(^2P_{3/2})5s$ states from inelastic-scattering measurements using electron-energy-loss spectroscopy. Most of the theoretical calculations of the GOS for many-electron atoms use an independent-particle model [3]. Lack of sufficiently accurate wave functions often limits the accuracy of the results obtained. In the present calculations, a recently developed relativistic local-density-potential method [4], referred to as the $RC\Xi$ method, has been employed for generating the ground-state and the excited-state wave functions. In this method, a local-density approximation is made to the many-electron potential and furthermore a part of the Coulomb correlation energy is accounted for using the "Coulomb hole" [4-6]. This method has been used with success for the calculation of the expectation value of r^n ($n = -1, 1, 2$), spin-orbit parameters, ionization energy, and electron affinity for various atoms [4]. The present work has been undertaken with the following two objectives:

(i) To test if the $RC\Xi$ potential is suitable to describe atomic-collision processes, since no prior study of collision phenomena has been attempted using this poten-

tial; and (ii) to examine the outcome of theoretical calculations of electron-atom (Kr, Xe) GOS in the context of the above-mentioned experiments [2].

For the sake of completeness, the $RC\Xi$ potential method has been described briefly in Sec. II. The well-known theory of Bethe [7,8] has been used for the determination of the GOS in the first-order Born approximation. A computer code developed by Manson [9] has been used to calculate these collision parameters. A brief account of the various approximations employed in our calculations of GOS is given in Sec. III. The results obtained are presented and discussed in Sec. IV, which is followed by concluding remarks in Sec. V.

II. THE RELATIVISTIC LOCAL-DENSITY METHOD

The Dirac Hartree-Fock (DHF) method developed by Grant [10,11] and Desclaux [12] is based on a relativistic reformulation of the Hartree-Fock self-consistent-field (HF-SCF) method [13,14]. This method makes use of the fully relativistic single-particle Dirac Hamiltonian and treats exchange exactly. To simplify the relativistic many-electron calculations, the exchange interaction may be approximated as in the nonrelativistic case by using Slater's local-density approximation [15]. Vaidehi and Gopinathan [16] proposed a parameter-free model in which the self-interaction is evaluated explicitly and a local-density approximation is made to the residual nonlocal-exchange term. The one-electron equations of this method were derived from the Dirac Hartree-Fock central field radial equations. The small components of the Dirac spinor are neglected in comparison with the

large components. The second-order differential equation obtained for the large component has the following form (in Rydberg units):

$$\left[-\frac{d^2}{dr^2} + \frac{l(l+1)}{r^2} + v(r) + H_m(r) + H_D(r) + H_{s.o.}(r) \right] P_{nlj}(r) = \epsilon_{nlj} P_{nlj}(r), \quad (1)$$

where

$$v(r) = -\frac{2Z}{r} + v^c(r) + v^{SI}(r) + v_i^{\text{exch}}(r),$$

$$v^c(r) = \sum_j n_j \int u_j^*(\mathbf{r}') u_j(\mathbf{r}') \frac{2}{|\mathbf{r} - \mathbf{r}'|} d\mathbf{r}',$$

$v^{SI}(r)$ is the self-interaction potential

$$v^{SI}(r) = -n_i \int u_i^*(\mathbf{r}') u_i(\mathbf{r}') \frac{2}{|\mathbf{r} - \mathbf{r}'|} d\mathbf{r}',$$

and $v_i^{\text{exch}}(r)$ is the pure exchange potential, discussed below. Also,

$$H_m(r) = -K[\epsilon - v(r)]^2,$$

$$H_D(r) = -KB \frac{dv}{dr} \left[\frac{d}{dr} - \frac{1}{r} \right],$$

$$H_{s.o.}(r) = -KB \left[\frac{\kappa+1}{r} \right] \frac{dv}{dr},$$

$$K = \frac{\alpha^2}{4}, \quad B = \left[1 + \frac{\alpha^2}{4} [\epsilon - v(r)] \right]^{-1},$$

$\kappa = -(j + \frac{1}{2})a$ and $a = \pm 1$, depending on $j = l \pm \frac{1}{2}$, and α is the fine structure constant.

The Fermi correlation between electrons of like spin keeps them apart and hence the Coulomb correlation between electrons of like spin is much less important compared to what it is for electron pairs of unlike spin. Accordingly in the present formalism Coulomb correlation between electrons of like spin is ignored. Coulomb correlation between electrons of unlike spin is included in the present method using a term similar to the one representing the "Fermi hole" of the local-density HF method [15]. The analogous entity, referred to as the "Coulomb hole" [4-6], is introduced in the present formalism and is required to have the following properties.

(i) The Coulomb hole density should satisfy Kato's cusp condition [5]. The solutions of the Schrödinger equation should exhibit a singularity at the position of the Coulomb singularity about which the Coulomb hole is centered. According to Kato, the wave function should have a sharp cusp at the positions of the Coulomb singularities ($r_{ij} = 0$).

(ii) The total Coulomb hole charge is zero, i.e., the Coulomb hole density integrates to zero over the entire range of the Coulomb hole [6]. Short-range correlation effects are included in this method partially by imposing the condition that the wave function should have a sharp cusp at the position of the Coulomb singularities. This is

achieved analytically by introducing interelectronic variables. This method is well suited for the determination of total energies. The total energy expression is written in this method with additional terms to include the Coulomb correlation effects:

$$\begin{aligned} \langle E \rangle = & \sum_i \int n_i u_i^*(\mathbf{r}) f_{1i} u_i(\mathbf{r}) d\mathbf{r} + \frac{1}{2} \int \rho(\mathbf{r}) \rho(\mathbf{r}') g_{rr'} d\mathbf{r} d\mathbf{r}' \\ & + \frac{1}{2} \int \rho_{\uparrow}(\mathbf{r}) U_{\uparrow}^{\text{ex}}(\mathbf{r}) d\mathbf{r} + \frac{1}{2} \int \rho_{\downarrow}(\mathbf{r}) U_{\downarrow}^{\text{ex}}(\mathbf{r}) d\mathbf{r} \\ & + \frac{1}{2} \int \rho_{\uparrow}(\mathbf{r}) U_{\uparrow}^{\text{corr}}(\mathbf{r}) d\mathbf{r} + \frac{1}{2} \int \rho_{\downarrow}(\mathbf{r}) U_{\downarrow}^{\text{corr}}(\mathbf{r}) d\mathbf{r}. \quad (2) \end{aligned}$$

In the above equation,

$$f_{1i} = -\nabla^2 - \frac{2Z}{r}, \quad \rho(\mathbf{r}) = \rho_{\uparrow}(\mathbf{r}) + \rho_{\downarrow}(\mathbf{r});$$

$$\rho_{\uparrow}(\mathbf{r}) = \sum_i n_i u_{i\uparrow}^*(\mathbf{r}) u_{i\uparrow}(\mathbf{r}), \quad g_{rr'} = \frac{2}{|\mathbf{r} - \mathbf{r}'|},$$

and $U_{\uparrow}^{\text{corr}}(\mathbf{r})$ is the "Coulomb hole" correlation potential acting upon an up spin electron, the potential being produced by all the down spin electrons. The variational minimization of the total energy $\langle E \rangle$ with respect to the spin orbitals u_i leads to the one-electron equations:

$$\{f_{1i} + v^c(r) + v_{\uparrow}^{SI}(r) + v_{\uparrow}^{\text{ex}}(r) + v_{\uparrow}^{\text{corr}}(r)\} u_{i\uparrow}(r) = \epsilon_i u_{i\uparrow}(r). \quad (3)$$

Equation (3) differs from the HF equation by the presence of the last term within the bracket on the left-hand side. This term, $v_{\uparrow}^{\text{corr}}(r)$, is added to the potential $v(r)$ used in Eq. (1), to obtain the one-electron equations. Further, the pure exchange potential has been determined by defining a local-density potential using the important property that the total charge removed from the Fermi hole is zero. The radius of the exchange hole in this model is assumed to be the same as the Fermi hole radius [16]. The exchange density and the potential become positive beyond a certain distance, which is fixed in terms of the Fermi hole radius. The exchange potential is then given by

$$\begin{aligned} U_{i\uparrow}^{\text{ex}}(\mathbf{r}) = & -4\pi^{1/3} (2^{1/3} - 1) \left[\frac{1}{n_{\uparrow}} + \frac{1}{3} \right]^{-2/3} \\ & \times \sum_j \rho_{j\uparrow}(\mathbf{r}) \rho_{\uparrow}^{-2/3}(\mathbf{r}) n_j u_j^*(\mathbf{r}) u_j(\mathbf{r}). \quad (4) \end{aligned}$$

It is the weighted average over all the occupied up spin orbitals. In Eq. (4), n_{\uparrow} is the total number of up spin electrons, $\rho_{\uparrow}(\mathbf{r})$ is the density of up spin electrons at the point \mathbf{r} , and $\rho_{j\uparrow}(\mathbf{r})$ is the density of up spin electrons excluding the i th electron.

A similar procedure is used for the determination of the Coulomb correlation potential. The Coulomb correlation for an electron of a given spin can be thought of as arising due to the removal of charge of all electrons having opposite spin from its vicinity. For small r , the Coulomb correlation potential is assumed to vary slowly. The Coulomb correlation potential for an electron of up spin at \mathbf{r} is given as

$$U_{\uparrow}^{\text{corr}}(\mathbf{r}) = -\frac{8\pi}{27} r_{c\uparrow}^3 \frac{\rho_{\downarrow}(\mathbf{r})}{(1+r_{c\uparrow})}. \quad (5)$$

The radius of the Coulomb hole is assumed to have the same functional dependence on the charge density as does the Fermi hole radius. It is considered to be given by

$$r_{c\uparrow}(\mathbf{r}) = x r_{F\downarrow}(\mathbf{r}),$$

where the Fermi hole radius

$$r_{F\downarrow}(\mathbf{r}) = \left[\pi \left[\frac{1}{n_{\downarrow} + \frac{1}{3}} \right] \rho_{\downarrow}(\mathbf{r}) \right]^{-1/3} \quad (6)$$

and the unknown x is fixed semiempirically [4].

This method of generating atomic potentials is referred to as the $RC\Xi$ method in literature. This name signifies the inclusion of relativistic and Coulomb correlation effects and an approximated exchange potential which is free from the well-known defects of the Hartree-Slater potential.

Expressions (4) and (5) are substituted in Eq. (2) for the total energy and the one-electron equations are determined by variational minimization. The final one-electron SCF equations of the $RC\Xi$ method turn out to be

$$\left\{ \left[-\frac{d^2}{dr^2} + \frac{l(l+1)}{r^2} - \frac{2Z}{r} + v^c(r) + v_{\uparrow}^{\text{SI}}(r) + v_{i\uparrow}^{\text{ex}}(r) + v_{\uparrow}^{\text{corr}}(r) \right] - \frac{\alpha^2}{4} [\varepsilon_{nlj} - v(r)]^2 \right. \\ \left. - \frac{\alpha^2}{4} \left[1 + \frac{\alpha^2}{4} [\varepsilon_{nlj} - v(r)] \right]^{-1} \frac{dv}{dr} \left[\frac{1}{P_{nlj}} \frac{dP_{nlj}}{dr} - \frac{1}{r} \right] - \frac{\alpha^2}{4} \left[1 + \frac{\alpha^2}{4} [\varepsilon_{nlj} - v(r)] \right]^{-1} \frac{dv}{dr} \Lambda \frac{1}{r} \right\} P_{nlj}(r) = \varepsilon_{nlj} P_{nlj}(r), \quad (7)$$

where Λ is $(l+1)$ for $j=l+\frac{1}{2}$ and $(-l)$ for $j=l-\frac{1}{2}$, and

$$v(r) = -\frac{2Z}{r} + v^c(r) + v_{\uparrow}^{\text{SI}}(r) + v_{i\uparrow}^{\text{ex}}(r) + v_{\uparrow}^{\text{corr}}(r). \quad (8)$$

The set of Coulomb correlated and relativistic one-electron equations (7) can be solved for atoms using a modified Herman-Skillman computer program [17] which performs spin-polarized calculations. The orbitals $\{u_i\}$ are not orthogonal since the orthogonalization constraint has not been included in the variational minimization scheme in order to keep the formalism simple. Nevertheless, orthogonality of the spin orbitals can be obtained subsequently using Lowdin's orthogonalization procedure [18] at each iteration of the SCF cycle [4].

III. THE METHOD FOR GOS CALCULATIONS

In the present work the GOS has been determined in the first-order Born approximation. For an N -electron atom described using a single-particle model, the expression for the GOS $f_n(K)$ for the excitation from an initial state Ψ_0 to a final state Ψ_n at excitation energy E_n measured from state 0 with momentum transfer $\hbar K$ is given [9] by

$$f_n(K) = \frac{E_n}{R} \frac{1}{(Ka_0)^2} |I_n(\mathbf{K})|^2, \quad (9)$$

in which the matrix element $I_n(\mathbf{K})$ is given by

$$I_n(\mathbf{K}) = \sum_{j=1}^N \int \Psi_n^* e^{i\mathbf{K}\cdot\mathbf{r}_j} \Psi_0 d\mathbf{r}_1 d\mathbf{r}_2 \cdots d\mathbf{r}_N, \quad (10)$$

where \mathbf{r}_j is the position vector of the j th atomic electron and a_0 is the Bohr radius. The matrix element in Eq. (9) will be independent of the azimuthal angle ϕ , when the state 0 is spatially symmetric or when the atoms under

study are oriented at random. In the latter case, an average over all atomic orientations is implied. Moreover, the term "state n " is often used to mean a set of all substates at E_n in which case the sum over these degenerate substates is also implied in Eq. (10). In the above circumstances, $I_n(K)$ will be a function of the scalar variable K , which is more convenient than ϑ for the study of the GOS. Such a simplification, however, cannot be made when spin-polarized atoms are used or when polarization of light from excited atoms is studied.

The cross section σ_n for excitation of an atom to a state n is obtained by integrating the above expression for $f_n(K)$,

$$\sigma_n = \frac{4\pi a_0^2 z^2}{(E_n/R)(v/v_0)^2} \int f_n(K a_0) d[\ln(K a_0)^2], \quad (11)$$

where v is the velocity of the incident particle, v_0 the Bohr velocity, and ze is the charge of the incident particle, e being the electronic charge. The GOS as well as the limits of integration $[\ln(K_{\text{max}} a_0)^2 \text{ and } \ln(K_{\text{min}} a_0)^2]$ in Eq. (11) depend on the excitation energy E_n . The upper and lower limits of integration are related to the initial and final wave numbers through the following relations:

$$K_{\text{max}} a_0 = (k_0 + k_n) a_0 \quad \text{and} \quad K_{\text{min}} a_0 = |k_0 - k_n| a_0.$$

At the threshold for excitation, the upper and lower limits are identical and it follows [19] that

$$(K_{\text{max}} a_0)^2 = (K_{\text{min}} a_0)^2 = \frac{M}{m_e} \left[\frac{E_n}{R} \right],$$

where M is the mass of the target atom and m_e is the mass of the electron. When the collision energy T is much higher than the excitation energy E_n ($E_n/T \ll 1$) the following approximate relations are valid:

$$K_{\max} a_0 \approx \frac{(2Mv)}{(m_e v_0)}, \quad (12a)$$

$$K_{\min} a_0 \approx \frac{E_n/R}{2(v/v_0)}. \quad (12b)$$

The errors arising due to such an approximation are small for ion-atom collision calculations [19].

To evaluate the integral in Eq. (10) the plane-wave part $e^{i\mathbf{K}\cdot\mathbf{r}}$ is expanded in terms of spherical Bessel functions:

$$e^{i\mathbf{K}\cdot\mathbf{r}} = \sum_{\lambda} i^{\lambda} (2\lambda+1) j_{\lambda}(Kr) P_{\lambda}(\cos\vartheta), \quad (13)$$

where ϑ is the angle between \mathbf{K} and \mathbf{r} , P_{λ} is the Legendre polynomial of order λ , and j_{λ} is the spherical Bessel function of order λ . The absolute square of the transition matrix element for an $nl \rightarrow n'l'$ transition is given by

$$|J_{nl,n'l'}|^2 = (2l'+1) \sum_{\lambda} (2\lambda+1) (R_{nl,n'l'}^{\lambda})^2 \left| \begin{matrix} l' & \lambda & l \\ 0 & 0 & 0 \end{matrix} \right|^2, \quad (14)$$

where

$$R_{nl,n'l'}^{\lambda} = \int_0^{\infty} P_{nl}(r) j_{\lambda}(Kr) P_{n'l'}(r) dr. \quad (15)$$

The sum over λ in Eq. (13) goes from $|l-1'|$ to $(l+1')$ in steps of 2 since the $3j$ symbol vanishes for all other values of λ .

Calculations of the GOS were performed using two different local-density potentials: (i) The Hartree-Slater (HS) potential [17]. The excited-state wave functions were generated in the HS potential using a computer code written by Manson. Relativistic effects and core relaxation effects were ignored in these calculations; and (ii) the $RC\Xi$ potential, described in Sec. II.

IV. RESULTS AND DISCUSSION

GOS calculations have been performed for excitation of krypton to the $4p^5(^2P_{1/2})5s$, $4p^5(^2P_{3/2})5s$ states and for the excitation of xenon to the $5p^5(^2P_{1/2})6s$, $5p^5(^2P_{3/2})6s$ states. The results are presented in Figs. 1(a) and 1(b) and 2(a) and 2(b), respectively, for Kr and Xe. All the figures contain the GOS results for both the potentials mentioned above. The nonrelativistic HS GOS has been factored in the proportion $\frac{1}{3}:\frac{2}{3}$ to get the HS estimates, respectively, for $np_{1/2} \rightarrow (n+1)s$ and the $np_{3/2} \rightarrow (n+1)s$ transitions, n being 4 for Kr and 5 for Xe. In a separate calculation, the $RC\Xi$ wave functions were determined by excluding the ‘‘Coulomb hole’’ correlation effects. The GOS values obtained by using these wave functions are also presented in Figs. 1 and 2 for each of the excitations considered. Also, the calculations were repeated after omitting the relativistic terms in the $RC\Xi$ potential to examine their contribution.

In Fig. 1(a), the experimental results of Takayanagi *et al.* [2] on krypton are also shown. The excitation energy E_n corresponding to this excitation $4p^5(^2P_{1/2})5s$ in the HS calculation was 0.696 Ry. In the $RC\Xi$ calculation, $E_n = 0.947$ Ry when ‘‘Coulomb hole’’ correlation is

included, and 0.915 Ry when it is excluded. In both the HS and the $RC\Xi$ potentials, the excitation energies have been calculated as the difference in orbital energies of the initial- and final-state levels involved in respective transitions.

Figure 1(b) gives the corresponding results for the excitation of krypton to the $4p^5(^2P_{3/2})5s$ state. The excitation energies for this transition using the $RC\Xi$ potential are $E_n = 0.890$ Ry when ‘‘Coulomb hole’’ correlation is included and $E_n = 0.858$ Ry when it is excluded. The experimental excitation energies for the $4p^5(^2P_{1/2})5s$ and $4p^5(^2P_{3/2})5s$ excitations are, respectively, ~ 0.783 and ~ 0.738 Ry.

A distinct minimum is found to occur at $(Ka_0)^2 \simeq 1.21$ in the calculations involving both the HS and the $RC\Xi$ potentials for both the excitations of krypton. It may be pointed out that Kim *et al.* [20] had predicted this minimum from their HF calculations.

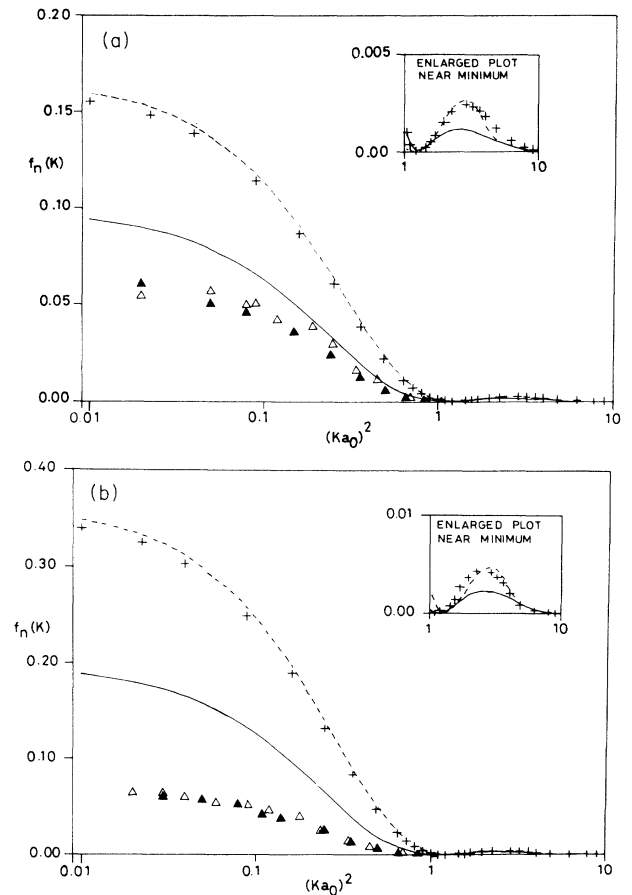


FIG. 1. Generalized oscillator strengths for the excitation of krypton to the (a) $4p^5(^2P_{1/2})5s$ state and (b) $4p^5(^2P_{3/2})5s$ state. —, result of the present calculation using the Hartree-Slater potential for the atom; ---, result of the present calculation using the $RC\Xi$ potential for the atom; +, result of the present calculation using the $RC\Xi$ potential for the atom when ‘‘Coulomb hole’’ correlation effects are omitted; Δ , experimental result of Takayanagi *et al.* [2] at 300-eV electron-impact energy; \blacktriangle , experimental result of Takayanagi *et al.* [2] at 500-eV electron-impact energy.

The results for excitation of xenon to the $5p^5(^2P_{1/2})6s$ state are given in Fig. 2(a). No experimental results are available for comparison in this case. The excitation energy for this transition is 0.604 Ry in the HS calculation. In the $RC\Xi$ calculation, $E_n = 0.865$ Ry when "Coulomb hole" correlation is included and 0.834 Ry when it is excluded. A minimum in the GOS occurs at $(Ka_0)^2 \approx 0.9$ in the HS calculation. In the $RC\Xi$ calculation, the minimum occurs at $(Ka_0)^2 \approx 1.0$.

The results for excitation of xenon to the $5p^5(^2P_{3/2})6s$ state are shown in Fig. 2(b). The HS result for this excitation was already reported by Manson [9]. The $RC\Xi$ excitation energy is 0.753 Ry when "Coulomb hole" correlation is included and 0.724 Ry when it is excluded. The minimum in the GOS occurs at the same value of momentum transfer as in the $5p^5(^2P_{1/2})6s$ excitation, since the HS calculations do not distinguish the level splittings. Kim *et al.* [20] predict the minimum at the same value from their HF calculation. However, their experiments predict the minimum at $(Ka_0)^2 \approx 0.7$. The

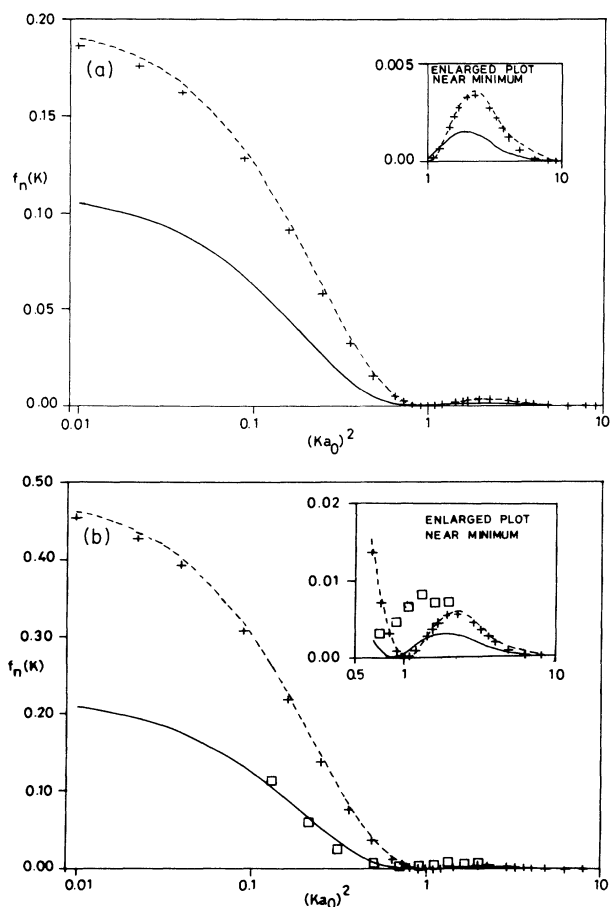


FIG. 2. Generalized oscillator strengths for the excitation of xenon to the (a) $5p^5(^2P_{1/2})6s$ state and (b) $5p^5(^2P_{3/2})6s$ state. —, result of the present calculation using the Hartree-Slater potential for the atom; ---, result of the present calculation using the $RC\Xi$ potential for the atom; +, result of the present calculation using the $RC\Xi$ potential for the atom when "Coulomb hole" correlation effects are omitted; □, experimental results of Kim *et al.* [20].

minimum in the GOS occurs at $(Ka_0)^2 \approx 1.1$ in the $RC\Xi$ calculations.

The results of the $RC\Xi$ calculations, without the "Coulomb hole" correlations, show that the contribution from these effects is negligible. Also, exclusion of relativistic terms in these calculations did not lead to any significant change in the results for the $np^5(^2P_{1/2})(n+1)s$ transition ($n=4$ for Kr and 5 for Xe) but the resulting GOS was slightly less for the $np^5(^2P_{3/2})(n+1)s$ excitation when relativistic effect was suppressed from the $RC\Xi$ calculation.

The minimum in the GOS occurs when the radial integrals in Eq. (14) pass through a minimum. For $p^6 \rightarrow p^5s$ transition the term in $\lambda=1$ alone contributes to the sum in Eq. (13) and hence the minimum occurs when the radial integral

$$\int P_{n_l}(r)j_1(Kr)P_{n_f}(r)dr$$

of Eq. (15) passes through a minimum. This happens for such a value of K when the first node of $j_1(Kr)$ coincides with the last node of the product $P_{n_l}(r)P_{n_f}(r)$, and the above integral has roughly equal positive and negative areas which tend to cancel each other. The existence of a minimum also depends on the angular momentum of the target states [21]. For example, when one of the target states is not an s state, for the simplest case of $\min(l_i, l_f) = 1$, two radial integrals must go through a minimum simultaneously for the same value of K . The situation becomes more complicated for higher values of $\min(l_i, l_f)$. The position of the minimum in the GOS depends on two factors, viz., the values of the radial integral and the excitation or ionization energies.

In the case of continuum transitions, there is a continuous succession of such minima for different E which form a trajectory on the plane with axes E/R and $\log_{10}(Ka_0)^2$ and hence a trough appears in the Bethe surface [22] which results from a three-dimensional plot of df/dE as a function of E and $\log_{10}(Ka_0)^2$ employed as independent orthogonal axes. If a trough reaches the $K=0$ plane, the optical limit, it appears as the well-known Cooper minimum (a minimum of the optical oscillator strength) [23]. It may be added that minimum (possibly a zero)/minima in the oscillator strength can be due to a variety of reasons [24]. Generally, the minimum is not a zero, as has been discussed in the case of the "Cooper minimum" [25,26].

For krypton, experimental data are available [2] only for $(Ka_0)^2 \leq 1$. The minimum found in the present calculations is not seen in the experimental results of Takayanagi *et al.* It will be interesting if experiments at higher values of momentum transfer are carried out to verify if the minimum in the GOS predicted by the present calculations is indeed observed.

It is to be remembered that the minimum in the GOS may not explicitly manifest itself in the scattering cross section. The cross section for excitation varies with the energy dependence of the upper and lower limits of integration [Eqs. (12)], in addition to its dependence on the GOS as a function of $\log_{10}(Ka_0)^2$. For large excitation energies, the upper limit of integration is well beyond the

value of the momentum transfer at which the minimum occurs in the GOS and hence a change in the upper limit does not significantly affect the integral cross section. The energy dependence of the integral cross section is therefore mainly due to the change in the lower limit of integration. The lower limit for electron impact is small [19] due to the small ratio of the electron to target atom mass. This ratio is large for ion-atom collisions. It has been shown by Iwai, Shimamura, and Watanabe [19] using plane-wave Born approximations for the case of $N^{3+}(2s^2\ ^1S \rightarrow 2s3p\ ^1P)$ excitation that the ion-impact excitation cross section does indeed go through a minimum, whereas the electron-impact cross section does not. It will be interesting if ion-impact excitation experiments are carried out to verify the present results.

Finally, it may be observed that the $RC\Xi$ results for GOS are higher than the HS results. One possible reason for this is the different manner in which the exchange potential is treated in these two models. Another reason is the fact that the $RC\Xi$ excitation energies are higher than the corresponding HS values. The excitation energy appears as a multiplication factor in the expression for the GOS [Eq. (9)] and thus causes an enhancement of the $RC\Xi$ results over the HS results. Furthermore, while it is generally known that relativistic effects cause the radial functions to become compact, different orbitals in a self-consistent field of a many-electron atom respond in different quantitative and even different qualitative ways to relativistic effects [27]. We compared the initial-state np and the final-state $(n+1)s$ orbitals calculated in the relativistic $RC\Xi$ and the nonrelativistic HS model potentials and found that the *excited-state* $(n+1)s$ orbitals are *relatively* more compact in $RC\Xi$ compared to the *initial-state* (np) orbitals. This would allow an enhanced overlap

and consequently an enhanced GOS in the $RC\Xi$ model relative to the HS model.

V. CONCLUSIONS

Within the validity of the Born approximation, the position of the minimum is related to the nodes of the orbitals of the electron active in the transition. The calculations reported here thus provide a stringent test of the wave functions calculated using the $RC\Xi$ method. The results of the present calculations suggest that the $RC\Xi$ method is well suited for studying atomic-collision processes. Since the $RC\Xi$ potential was used in separate calculations using different levels of approximation, it is possible to conclude that the results of these calculations are not significantly sensitive to "Coulomb hole" correlation effects but are somewhat sensitive to the relativistic effects. The differences in the HS and $RC\Xi$ results are also caused by the different treatment of the exchange interactions in the two models. We have undertaken several additional collision studies to examine these factors in further detail.

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