Relativistic Configuration Interaction Treatment of Generalized Oscillator Strength for Krypton *

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(Received 27 April 2007)

A fully relativistic configuration interaction method is developed to investigate the transition energies and general oscillator strengths of the lower lying states of krypton, for both optically allowed and optically forbidden transitions. The calculated results are in agreement with the recent experimental measurements. The calculated transition energies for the $5s$ and $5s'$ transitions are 9.970 and 10.717 eV, which agree with the experimental data of 10.033 and 10.643 eV. The calculated oscillator strengths are 0.211 and 0.170, comparable with the experimental results 0.214(±0.012) and 0.194 (±0.012), respectively. The momentum transfer positions (K^2 in a.u.) of the minimum and maximum GOSs in the $4s^24p^6 \to 4s^24p^5$ $(5s + 5s')$ transitions are 1.105 and 2.225, comparable with the measurements results 1.24 and 2.97 [Phys. Rev. A **67** *(2003) 062708].*

PACS: 34. 80. Dp, 31. 25. Jf, 31. 30. Jv

Electron-impact cross sections of atomic krypton are widely used in plasma diagnostics for the thermonuclear reactor, plasma processing in flat-panel display technology, pumping mechanisms in Kr laser systems.[1]

Recently, the absolute generalized oscillator strengths (GOS) for transitions from the ground state of Kr to the excited states $5s$, $5s'$, and $5p$ were measured at electron energy of 2.5 keV, the minimum and maximum positions of these GOSs were also determined.[2] This can be used as a benchmark to test the theoretical calculations.

In theory, the relativistic methods, such as multiconfiguration relativistic Hartree–Fock (MCRHF)[3] and multiconfiguration Dirac–Fock (MCDF),[4] can be utilized to study the structure and dynamics for middle- and high-Z atomic systems. In this Letter, we develop a fully relativistic configuration interaction (RCI) method to calculate GOSs, in which the orbital wavefunctions are calculated by using the Dirac–Slater self-consistent field (SCF) method.[5] The atomic wavefunctions, transition energies and GOSs are obtained by employing a configuration interaction method.[6] To elucidate the validity of this method, the transition energies and GOSs of the lower lying states of Kr are calculated for both optically allowed and optically forbidden transitions. The calculated results are in agreement with the experimental measurements[2] and other theoretical works.

The RCI method has been described in the literature.[6] Here we only briefly discuss the main points. The single electron orbitals

$$\varphi_\eta = \frac{1}{r}\begin{pmatrix} G_n(r) & Y_{ljm} \\ iF_n(r) & Y_{ljm} \end{pmatrix}$$

can be obtained from the Dirac–Slater SCF method[7] with the Hamiltonian

$$H_0 = \sum [c\alpha_i P_i + \beta_i mc^2 + V^{(i)}_{\rm rscf}],$$

where $V^{(i)}_{rscf}$ is the SCF potential. The orbitals are used to construct the anti-symmetrized product-type configuration wavefunctions Ψ_i of the atomic system with appropriate angular moment coupling and electron occupation distribution. These configuration wavefunctions form a basis set of the complete Hilbert space of the atomic system $\{\Psi_i\}$. The atomic state wavefunctions are the linear superpositions of the configuration wavefunctions,

$$\Psi = \sum C_i \Psi_i.$$

The superposition coefficients C_i can be calculated by diagonalizing the corresponding Hamiltonian matrix, and then the atomic energies and wavefunctions can be obtained.

With the atomic energies and wavefunctions, the generalized oscillator strengths of the atomic system can be calculated as

$$f(E,K) = \frac{EK^2}{2}\frac{p_0}{p_a}\frac{d\sigma}{d\Omega} = \frac{2E}{K^2}|\langle\Psi_f|\sum_{j=1}^{N} e^{i\boldsymbol{K}\cdot\boldsymbol{r}_j}|\Psi_i\rangle|^2,$$

where $f(E,K)$ and $d\sigma/d\Omega$ represent the GOS and differential cross section; E and K are the excitation energy and momentum transfer, while p_0 and p_a are the incident and scattered electron momenta, respectively; Ψ_i and Ψ_f are the initial and final N-electron atomic wavefunctions; $\boldsymbol{r}_j$ is the position vector of the

* Supported by the Scientific Research Foundation for the Returned Overseas Chinese Scholars, State Education Ministry, and the Scientific Research Fund of Graduate University of the Chinese Academy of Sciences under Grant No 055101BM03.

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jth electron. The detailed formula can be found in Refs. [5,6]

The ground-state configuration of Kr is [Ar] $3d^{10}4s^24p^6$. Only one- and two-electron excitations from $4s$ and $4p$ orbitals are included in the present calculation with other electrons considered as a frozen core, i.e. the configurations $4s^24p^5np$, $4s4p^6n's$, $4s^24p^45sn's/nd$, $4s4p^55sn'p/n''f$, $4s^24p^45pn'p/n''f$ and $4s^24p^45pn's/n''d$ are used for the total angular momentum $J = 0$ in even parity, the configurations $4s^24p^5n's/nd$, $4s4p^6n'p/nf$, $4s^24p^45sn'p/n''f$, $4s4p^55sn's/nd$, $4s^24p^45pn's/nd$ and $4s4p^55pnp/n''f$ for $J = 1$ in odd parity, and the configurations $4s^24p^5n'p$, $4s4p^6nd$, $4s^24p^45sn's/nd$, $4s4p^55sn'p/n''f$, $4s^24p^45pn'p/n''f$ and $4s4p^55pn's/n''d$ for $J = 2$ even parity. In our calculations, we choose ($4 \le n \le 8$, $5 \le n' \le 8$, $4 \le n'' \le 5$). Here a non-relativistic notation is used for simplicity, e.g. $4p^5$ denotes $4p_{1/2}^2 4p_{3/2}^3$ or $4p_{1/2}4p_{3/2}^4$, etc.

The calculated GOSs for optically allowed transitions $4s^24p^6 \to 4s^24p^55s/5s'$ are in agreement with the experimental results[2] as shown in Fig. 1.

The calculated transition energies for $5s$ and $5s'$ transitions are 9.970 and 10.717 eV, which are comparable with the experimental data of 10.033 and 10.643 eV,[8] and the errors are less than 1%. When $K \to 0$, GOSs approach the optical oscillator strength for optically allowed transitions. The calculated oscillator strengths ($K \to 0$) are 0.211 and 0.170, which agree with the experimental results 0.214 ($\pm$0.012) and 0.194 ($\pm$0.012),[8] respectively.

As the momentum transfer increases, there appears to be a minimum value of GOSs and then a maximum value. Our results agree with the experimental measurement[2] as shown in Fig. 1. The comparison of positions of the minimum and maximum for GOSs is listed in Table 1.

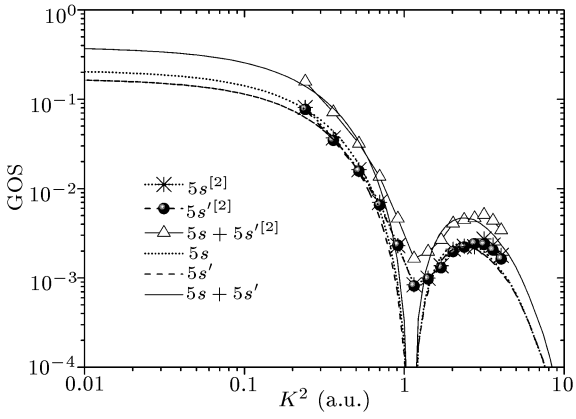


Fig. 1. Generalized oscillator strengths (GOSs) for the optically allowed transition $4s^24p^6 \to 4s^24p^55s/5s'$, i.e. the present theoretical results (lines) for the $5s$, $5s'$ and $5s+5s'$ transitions, and the experimental results (symbols) for $5s$, $5s'$ and $5s + 5s'$ transitions.[2]

Table 1. The momentum transfer positions (K^2 in a.u.) of the minimum and maximum GOS in the $4s^24p^6 \to 4s^24p^5(5s + 5s')$ transitions of krypton, compared with the experimental measurements and other theoretical calculations.

	Present	Expt[2]	Expt[9]	Expt[10]	Theory[9]	Theory[11]	Theory[12]
Minimum	1.105	1.24	0.90	1.04	1.21	0.69	1.053
Maximum	2.225	2.97		2.50		1.35	2.40

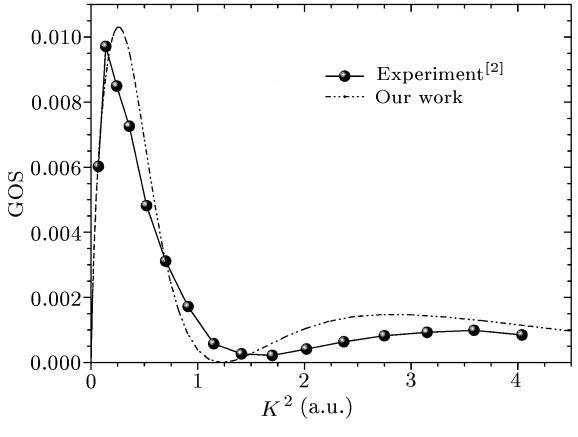


Fig. 2. GOSs for optically forbidden transition $4s^24p^6 \to 4s^24p^55p[5/2]_2$ (electric quadrupole).

In Table 1, there are some discrepancies among the theoretical and experimental data. The random-phase approximation with exchange effect and the Hartree–Fock approximation are used in Ref. [12]. The minimum and maximum of GOSs is slightly different from the measurements.[2] They shift to 1.25 and 2.50 after convolution,[2] which are closer to the experimental results.[2] The agreement between our results and the experimental data should also be improved after the convolution. The first Born approximation within one-electron approximation by employing scaled hydrogen-like orbitals in Ref. [11] cannot provide good results.

The calculated GOSs for optically forbidden transition $4s^24p^6 \to 4s^24p^55p[5/2]_2$ (electric quadrupole) are in general agreement with the experimental results,[2] as shown in Fig. 2. The calculated transition energy is 11.434 eV, comparable with the measured value of 11.445 eV.[8] There exist some discrepancies in the positions of the minimum and maximum of GOSs between the present calculations and the measurements. The reason is still unclear, because it is more difficulty to obtain accurate results in both theoretical and experimental works, for the optically forbidden process. The GOSs are more sensitive to the convergences of wave functions when their values are

smaller. Meanwhile, they also change more rapidly with the momentum transfer. Compared with the optically allowed transitions, these inevitably increase the difficulty in measurements. Further experimental and theoretical investigations are expected.

In summary, the present results show that our developed relativistic configuration interaction method is valid to calculate the transition energies and GOSs for both optically allowed and optically forbidden transitions. Due to fully relativistic treatment, the present RCI method can be applied to arbitrary atom systems.

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