Electron-impact excitation of Fe XXV and Kr XXXV in the relativistic distorted-wave approximation

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Cross sections for the electron-impact excitation of the $n = 2$ states of the heliumlike ions Fe XXV and Kr XXXV are calculated in the relativistic distorted-wave approximation. Both bound-core orbitals and continuum-scattering orbitals are calculated using the Dirac Hamiltonian. The most significant relativistic effects result from the spin-orbit mixing of the $2\,^3P_1$ and $2\,^1P_1$ excited states. We compare our results with previous calculations based on a perturbation-theory treatment of relativistic effects.

Among many applications, the knowledge of electron-ion impact excitation cross sections provides a basis for the interpretation of ultraviolet and x-ray emission from astrophysical and laboratory plasmas. Recently x-ray lines from Fe XXV impurity ions have been used to deduce temperatures in tokamak discharges.[1] For future experiments the determination of temperatures and densities will depend in part on the calculation of electron-impact excitation rates for other heavy atomic ions; in particular, perhaps the element krypton.[2]

For heavier atomic systems relativistic effects play an increasingly more important role. To obtain accurate electron-impact excitation rates one line of effort has made use of the Dirac-Fock Hamiltonian.[3] Powerful multiconfigurational bound-state methods have been developed[4] which now make routine the calculation of ground and excited states for the target atomic ion. The dynamical interaction of the scattering electron with the target ion may be treated by the multichannel eigenfunction expansion method.[5-8] Although a full solution of the close-coupled equations is quite difficult, in many cases (especially those involving highly charged atomic ions) a distorted-wave solution may achieve a reasonable level of accuracy.

In this paper we use a relativistic distorted-wave method based on the Dirac-Fock Hamiltonian to calculate transitions to the $n = 2$ states of the He-like ions Fe XXV and Kr XXXV. We use an undistorted final state form of the distorted-wave method.[9-11] The total wave function Ψ is expanded in a representation $(nJ_n\epsilon_n\kappa_n JM_J)$ in which the total angular momenta of the scattered electron (j_n) and the ion (J_n) are coupled together. The scattered electron energy, ϵ_n, takes the zero of the energy as the rest energy of the electron. The quantum number $\kappa_n = -(l_n + 1)$ if $j_n = l_n + \frac{1}{2}$ and $\kappa_n = l_n$ if $j_n = l_n - \frac{1}{2}$, where l_n is the orbital angular momentum of the scattered electron. One assumes that the total system angular momentum quantum numbers J and M_J, as well as parity Π, are conserved during the collision. The relativistic Hamiltonian, H, for the system is given by

$$H = \sum_{i=1}^{N+1} h_i + \sum_{i,j;\,\text{pairs}}^{N+1} v_{ij}\,, \tag{1}$$

where

$$h_i = c\vec{\alpha}\cdot\vec{p}_i + \beta c^2 + V_n(r)\,. \tag{2}$$

In Eqs. (1) and (2), $\vec{\alpha}$ and β are the usual Dirac matrices, the $\vec{p}_i$ are electron momenta, N is the number of electrons in the target, c is the speed of light, and atomic units are used. The nuclear potential, $V_n(r)$, includes effects due to the finite size of the nucleus.[4] The interaction between pairs of electrons, v_{ij}, is taken to be only the Coulomb part, $1/|\vec{r}_i - \vec{r}_j|$.

The two-component scattering orbital $[P^{\Gamma}_{\epsilon_i\kappa_i}(r), Q^{\Gamma}_{\epsilon_i\kappa_i}(r)]$ for the initial state, Ψ_i, may be determined from the Kohn variational principle, which is equivalent to

$$\langle \delta\psi_i^{\Gamma}|H - E|\psi_i^{\Gamma}\rangle = 0\,, \tag{3}$$

where the variation δ is made on the scattering orbital assuming no orthogonality restriction, and $\Gamma = J\Pi$ is a fixed set of conserved quantum numbers. The radial distorted-wave equation, found from Eq. (3), has the form

$$\begin{pmatrix} \frac{d}{dr} + \frac{\kappa_i}{r} & \frac{V_n}{c} + \frac{V_{ii}^{\Gamma}}{c} - 2c - \frac{\epsilon_i}{c} \\ \frac{V_n}{c} - \frac{V_{ii}^{\Gamma}}{c} + \frac{\epsilon_i}{c} & \frac{d}{dr} - \frac{\kappa_i}{r} \end{pmatrix} \begin{pmatrix} P^{\Gamma}_{\epsilon_i\kappa_i}(r) \\ Q^{\Gamma}_{\epsilon_i\kappa_i}(r) \end{pmatrix} = 0\,, \tag{4}$$

where the V_{ii}^{Γ} potential term symbolizes both direct and nonlocal exchange terms. The continuum

normalization is chosen such that

$$P^{\Gamma}_{\epsilon\kappa}(r) \xrightarrow[r\to\infty]{} \sin(pr + y\ln 2pr - \tfrac{1}{2}l\pi + \delta_\kappa)\,, \tag{5}$$

where the scattered electron momentum $p = (2\epsilon + \epsilon^2/c^2)^{1/2}$, $y = (Z-N)(\epsilon + c^2)/pc^2$, Z is the atomic number, and δ_κ is the phase shift.

The scattering orbital $[P^{\Gamma}_{\epsilon_f\kappa_f}(r), Q^{\Gamma}_{\epsilon_f\kappa_f}(r)]$ for the final state, Ψ_f, is found by solving Eq. (4) with the replacements $V^{\Gamma}_{ii} \to N/r$ and $\epsilon_i \to \epsilon_f$. The outgoing electron energy $\epsilon_f = \epsilon_i + \Delta E$, where ΔE is the excitation threshold energy.

Following standard nonrelativistic procedures,[11] the relativistic cross section σ for a transition $nJ_i \to n'J_f$ is given by

$$\sigma = \sum_{J\kappa_i\kappa_f} \sigma(\Gamma, \kappa_i \to \kappa_f)\,, \tag{6}$$

where

$$\sigma(\Gamma, \kappa_i \to \kappa_f) = \frac{8\pi(2J+1)}{p_i^3 p_f (2J_i+1)} \times \left(1 + \frac{\epsilon_i}{2c^2}\right)\left(1 + \frac{\epsilon_f}{2c^2}\right) |\langle \hat{\psi}_f^{\Gamma} | H' | \hat{\psi}_i^{\Gamma} \rangle|^2\,, \tag{7}$$

and $\hat{\psi}^{\Gamma}$ is a coupled product of the target ion state and the distorted-wave orbital $(P^{\Gamma}_{\epsilon\kappa}, Q^{\Gamma}_{\epsilon\kappa})$. The interaction Hamiltonian H' is given by[11]

$$H' = \sum_{i+1}^{N} v_{iN+1} - \frac{N}{r_{N+1}}\,. \tag{8}$$

TABLE I. Multiconfiguration Dirac-Fock calculations for target wave functions.

A. Energies and mixing coefficients for Fe XXV

Configuration	Threshold energy (a.u.)	Experimental energy [a] (a.u.)
$1s^2\,{}^1S_0$	0.00	0.00
$1s2\bar{p}\,{}^3P_0$	244.99	
$(a_1 1s2\bar{p} + a_2 1s2p)\,{}^3P_1$	245.12	245.17
$1s2p\,{}^3P_2$	245.67	245.57
$(b_1 1s2\bar{p} + b_2 1s2p)\,{}^1P_1$	246.33	246.28

Mixing coefficients

$a_1 = 0.9438$ $\quad b_1 = 0.3297$
$a_2 = -0.3306$ $\quad b_2 = 0.9441$

B. Energies and mixing coefficients for Kr XXXV

Configuration	Threshold energy
$1s^2\,{}^1S_0$	0.00
$1s2\bar{p}\,{}^3P_0$	478.80
$(a_1 1s2\bar{p} + a_2 1s2p)\,{}^3P_1$	479.09
$1s2p\,{}^3P_2$	481.44
$(b_1 1s2\bar{p} + b_2 1s2p)\,{}^1P_1$	482.29

Mixing coefficients

$a_1 = 0.9855$ $\quad b_1 = 0.1693$
$a_2 = -0.1696$ $\quad b_2 = 0.9856$

C. Oscillator strengths for Fe XXV

Transition	Length	Velocity	RRPA [b]
${}^1S_0 \to {}^3P_1$	0.059	0.058	0.066
${}^1S_0 \to {}^1P_1$	0.721	0.716	0.706

D. Oscillator strengths for Kr XXXV

Transition	Length	Velocity	RRPA
${}^1S_0 \to {}^3P_1$	0.144	0.143	0.159
${}^1S_0 \to {}^1P_1$	0.635	0.632	0.608

[a] Reference 12.
[b] Reference 13.

The initial and final states of the Fe XXV and Kr XXXV ions were calculated in the Dirac-Fock approximation. We used Desclaux's multiconfiguration Dirac-Fock computer code[4] to generate the target states $1s^2\,{}^1S_0$, $1s2\bar{p}\,{}^3P_0$, $(a_1 1s2\bar{p} + a_2 1s2p)\,{}^3P_1$, $1s2p\,{}^3P_2$, and $(b_1 1s2\bar{p} + b_2 1s2p)\,{}^1P_1$. Our orbital notation is such that $n\bar{l}$ is the $j = l - \frac{1}{2}$ state, while nl is the $j = l + \frac{1}{2}$ state. The mixing coefficients (a_i, b_i), energies, and oscillator strengths are given in Table I. We should note that the distorted-wave method used in this paper incorporates an ability to mix basis orbitals. The $1s$ orbital, for instance, is slightly different for each of the five target states. Our oscillator strengths in Table I are in fairly good agreement with the more accurate relativistic random-phase approximation (RRPA) values of Lin *et al.*[13] We used our calculated threshold energies, ΔE, in all subsequent cross section results.

Specific forms of the distorted-wave potential found in Eq. (4) and the transition integral found in Eq. (7) for He-like ion scattering may be readily derived for each partial wave.[3] For example, the $J = \frac{1}{2}$, $\epsilon_i s \rightarrow \epsilon_f \bar{p}$ partial wave for the $1\,{}^1S_0 \rightarrow 2\,{}^3P_1$ transition has

$$V_{ii}^{1/2} = 2J_{1s}^0 - K_{1s}^0 \,, \tag{9}$$

and

$$\begin{aligned}\langle \hat{\psi}_f^{1/2} | H' | \hat{\psi}_i^{1/2} \rangle = {} & (\tfrac{2}{27})^{1/2} a_1 \langle 2\bar{p}' \epsilon_f \bar{p} | v1 | 1s\epsilon_i s \rangle \langle 1s' | 1s \rangle \\ & + (\tfrac{1}{54})^{1/2} a_1 \langle \epsilon_f \bar{p} 2\bar{p}' | v1 | 1s\epsilon_i s \rangle \langle 1s' | 1s \rangle \\ & - (\tfrac{1}{6})^{1/2} a_1 \langle \epsilon_f \bar{p} 2\bar{p}' | v1 | 1s1s \rangle \langle 1s' | \epsilon_i s \rangle \\ & + (\tfrac{4}{27})^{1/2} a_2 \langle 2p' \epsilon_f \bar{p} | v1 | 1s\epsilon_i s \rangle \langle 1s' | 1s \rangle \\ & - (\tfrac{4}{27})^{1/2} a_2 \langle \epsilon_f \bar{p} 2p' | v1 | 1s\epsilon_i s \rangle \langle 1s' | 1s \rangle . \end{aligned} \tag{10}$$

The J_{nl}^v and K_{nl}^v terms in Eq. (9) symbolize direct and exchange potentials,[3] while $\langle nl\epsilon l | v\nu | nl'\epsilon l' \rangle$ and $\langle nl | \epsilon l \rangle$ are the radial Coulomb matrix element and radial overlap integral, respectively.[3] One should note that $|\epsilon_f \bar{p}\rangle$ is calculated as a relativistic Coulomb wave and the primed orbitals belong to the final target state.

Our total cross section results for the excitation of the $n = 2$ states of Fe XXV and Kr XXXV are presented in Table II and Figs. 1 and 2. For the $\Delta n = 1$ transitions investigated here, the partial-wave series of Eq. (6) converges rapidly. For each of the four transitions we included all partial waves such that $J \leq \frac{13}{2}$. For the transition to the $2\,{}^3P_0$ state this meant a total of 14 partial-wave cross sections, to the $2\,{}^3P_1$ and $2\,{}^1P_1$ states this meant 40, while the $2\,{}^3P_2$ had 50. As pointed out recently by Callaway *et al.*,[14] numerical problems arise in the integration of Dirac wave functions at the larger angular momenta. These problems

TABLE II. Excitation cross sections (units cm^2).

A. Incident energy = 6.71 keV on Fe XXV

Transition	This work	M. Jones [a]	D. H. Sampson *et al.* [b]
$1\,{}^1S_0 \rightarrow 2\,{}^3P_0$	4.19^{-23} [c]	3.98^{-23}	3.96^{-23}
$1\,{}^1S_0 \rightarrow 2\,{}^3P_1$	1.44^{-22}	1.38^{-22}	1.44^{-22}
$1\,{}^1S_0 \rightarrow 2\,{}^3P_2$	1.98^{-22}	1.98^{-22}	2.00^{-22}
$1\,{}^1S_0 \rightarrow 2\,{}^1P_1$	3.67^{-22}	3.80^{-22}	4.24^{-22}

B. Incident energy = 9.20 keV on Fe XXV

Transition	This work	M. Jones	D. H. Sampson *et al.*
$1\,{}^1S_0 \rightarrow 2\,{}^3P_0$	1.91^{-23}	1.77^{-23}	1.77^{-23}
$1\,{}^1S_0 \rightarrow 2\,{}^3P_1$	8.79^{-23}	8.21^{-23}	8.93^{-23}
$1\,{}^1S_0 \rightarrow 2\,{}^3P_2$	8.92^{-23}	8.88^{-23}	8.88^{-23}
$1\,{}^1S_0 \rightarrow 2\,{}^1P_1$	4.38^{-22}	4.48^{-22}	4.91^{-22}

C. Incident energy = 13.90 keV on Kr XXXV

Transition	This work	D. H. Sampson *et al.*
$1\,{}^1S_0 \rightarrow 2\,{}^3P_0$	9.98^{-24}	9.04^{-24}
$1\,{}^1S_0 \rightarrow 2\,{}^3P_1$	4.46^{-23}	4.51^{-23}
$1\,{}^1S_0 \rightarrow 2\,{}^3P_2$	4.45^{-23}	4.53^{-23}
$1\,{}^1S_0 \rightarrow 2\,{}^1P_0$	9.40^{-23}	1.08^{-22}

[a] Reference 15.
[b] Reference 16.
[c] The superscript denotes the power of ten by which the entry is to be multiplied.

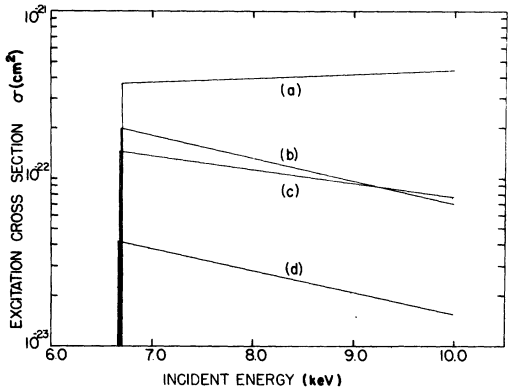

FIG. 1. Electron-impact excitation cross sections for the $n=2$ states of Fe XXV. Curve (a) is $1^1S_0 \rightarrow 2^1P_1$; curve (b) is $1^1S_0 \rightarrow 2^3P_2$; curve (c) is $1^1S_0 \rightarrow 2^3P_1$; curve (d) is $1^1S_0 \rightarrow 2^3P_0$.

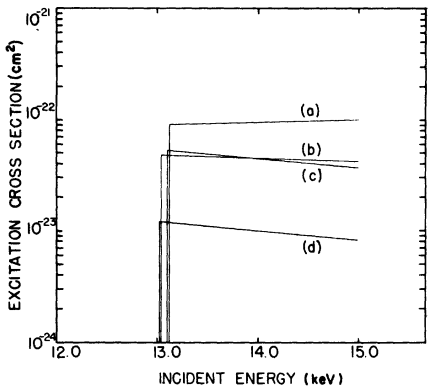

FIG. 2. Electron-impact excitation cross sections for the $n=2$ states of Kr XXXV. Curve (a) is $1^1S_0 \rightarrow 2^1P_1$; curve (b) is $1^1S_0 \rightarrow 2^3P_1$; curve (c) is $1^1S_0 \rightarrow 2^3P_2$; curve (d) is $1^1S_0 \rightarrow 2^3P_0$.

are not too significant here due to the rapid partial-wave convergence.

We compare our Fe XXV results in Table II at two different energies with the distorted-wave results of Jones[15] and the Z-expansion results of Sampson *et al.*[16] Both techniques used a Breit-Pauli perturbation treatment of relativistic effects to calculate the intermediate coupled transition rates. We also compare our Kr XXXV results in Table II at a single energy with the Z-expansion results.[16]

Since no experimental results are available for comparison, it is important to outline where systematic improvements may be made in our calculation. In regard to relativistic effects, we feel that the Dirac-Fock theory is the natural one to use when describing heavy atomic systems. In contrast to the usual Breit-Pauli perturbation treatments, the Dirac-Fock Hamiltonian includes certain relativistic effects, such as the spin-orbit interaction, in a completely nonperturbative manner. In regard to electron correlation effects, we may divide their contributions into two types.[17] The first type may be called core correlations or those correlations affecting the N-electron target states. As given in Table I, we found differences on a 2–5% level between oscillator strengths calculated in a single configuration approximation and those including correlations through the random-phase approximation. The second type may be called collisional correlations or those correlations arising from the solution of the multichannel dynamical problem. We must first ask to what accuracy the distorted-wave method solves the multichannel close-coupled equations. The distorted-wave method, of course, treats the off-diagonal coupling potentials as a perturbation. Barring degenerate or nearly degenerate excited states, experience has shown[18] that the distorted-wave method becomes more accurate as one goes to the higher-Z members of a given isoelectronic sequence. We must also ask to what degree resonances may enhance the average excitation cross section.[18,19] In our calculation for Fe XXV and Kr XXXV we have included only five open channels in our $(N+1)$ electron wave function expansion. The inclusion of energetically higher closed channels will undoubtedly lead to the appearance of resonance structures in Figs. 1 and 2. Although at particular resonance energies the cross section may be greatly enhanced, the average effects of resonances, as defined by Gailitis,[20] may in fact be quite small. We are currently engaged in extending the Dirac-Fock distorted-wave theory, as outlined above, to the calculation of resonance structures for heavy atomic ions. At the present time we thus urge caution in using results which are in fact only the nonresonant part of the inelastic cross section.

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