Relativistic Multiconfiguration Method In Elastic Low-Energy Scattering of Electrons From Xenon

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Introduction

In this work, we present the relativistic version of the multiconfiguration and configuration-interaction methods to describe the polarization of different target states due to the incoming electron charge through bound relativistic configuration expansions. The polarization is different for different kinetic energies of the scattering electron and thus dynamic effects are taken into account. The relativistic phase shifts obtained by this method are used to calculate spin-polarization and differential cross sections of the electron scattered by xenon in its ground state at a selected energies.

Computational Method

- In this study, wavefunctions have been generated by the widely–used atomic structure package **GRASP92** (Parpia, Froese Fischer & Grant, 1996). To represent the atomic ^1S ground-state function, 1081 relativistic configuration state functions (CSF) with total angular momentum $J = 0$ and even parity have been included. These CSF have been obtained by the excitations of one or two electrons from the $5s$ and $5p$ subshells into the set of virtual orbitals $\{6s\ 8d\ 10s$ and $10p\}$.

  Further relativistic contributions of the atomic states due to (transverse) Breit interactions were also added by diagonalizing the Dirac–Coulomb–Breit Hamiltonian matrix. The dominant QED contributions to the transition energies have also been included in the computations.
- These atomic orbitals have been used to construct $(N+1)$-electron configuration state functions by performing configuration-interaction calculations. Angular couplings of the atomic configuration state functions with the continuum orbitals and the numerical integrations of the continuum orbitals have been performed with a modified version of the computer code **COWF** (Fritzsche, in preparation). The original code has been modified to run on the multiprocessor machines (Dziedzic, Syty, Sienkiewicz, in preparation). The MPI method has been choosen to vectorize the code. The program has been run on the IA32 Xeon 700 (128 processors cluster) at the Academic Computer Center in Gdańsk TASK. This cluster is one of the powerfull machines in the Central Europe.
- Relativistic phase shifts have been calculated by comparing the numerical solutions of the Dirac–Fock equations, to the analytical ones at large r where $rV(r) \to 0$:

$$\frac{P_{n\kappa}(r)}{r} \sim j_l(kr)\cos\delta_l^{\pm} - n_l(kr)\sin\delta_l^{\pm}$$

  where k is the momentum of the scattered electron and j_l and n_l are the spherical Bessel and Neumann functions, respectively.
- We have calculated phase shifts of the elastic channel for $l = 0, 1, \ldots 6$. Then, using the nonrelativistic formula (Ali and Fraser, 1977), we have extended the calculations up to $l = 50$. After that, calculations of the spin polarization and differential cross sections have been performed.

References

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Theory

- Relativistic scattering equation: $H_{N+1}\Psi = \mathcal{E}\Psi$
- The $(N+1)$-electron Dirac–Coulomb Hamiltonian:

$$H_{N+1} = \sum_{i=1}^{N+1}\left[c\sum_{k=1}^{3}\alpha_i^k p_i^k + (\beta^i - 1)c^2 - \frac{Z}{r_i}\right] + \sum_{i<j}^{N+1}\frac{1}{r_{ij}}$$

- In the MCDF method, an atomic state is approximated by a linear combination of configuration state functions (CSF) of the same symmetry, so we describe the N-electron atomic states by this multiconfiguration expansion:

$$\Psi_a(PJM;N) = \sum_{r=1}^{n_c} c_r(a)\,|\gamma_r PJM\rangle$$

  In standard calculations, the CSF are antisymmetrized products of a common set of *orthonormal* orbitals which are optimized on the basis of the Dirac–Coulomb Hamiltonian.
- We define the $(N+1)$-electron scattering-state wave function as the coupled state of an N–electron wave function and a scattering-electron wave function:

$$\Psi(PJM;N+1) = \mathcal{A}\sum_{a=1}^{m_a} c_a\Psi_a(P_a J_a M_a;N)u_{\kappa(a)m(a)} + \sum_{j=1}^{m_d} d_j|\gamma_j PJM;N+1\rangle$$

  In our study, $m_a = 1$ (we examine only elastic scattering).
- The continuum Dirac spinor is defined as

$$u_{\kappa m}(\mathbf{r}) = \frac{1}{\mathbf{r}}\begin{pmatrix} P_{n\kappa}(r) & \chi_{\kappa m}(\mathbf{r}/r) \\ \mathrm{i}Q_{n\kappa}(r) & \chi_{-\kappa m}(\mathbf{r}/r)\end{pmatrix}$$

  where $P_{n\kappa}$ and $Q_{n\kappa}$ refer to continuum orbitals.
- The continuum orbitals are solutions of the Dirac–Fock equations:

$$\left(\frac{\mathrm{d}}{\mathrm{d}r} + \frac{\kappa}{r}\right)P_{n\kappa}(r) - \left(2c - \frac{E}{c} + \frac{Y(r)}{cr}\right)Q_{n\kappa}(r) = -\frac{\chi^{(P)}(r)}{r}$$
$$\left(\frac{\mathrm{d}}{\mathrm{d}r} - \frac{\kappa}{r}\right)Q_{n\kappa}(r) + \left(-\frac{E}{c} + \frac{Y(r)}{cr}\right)P_{n\kappa}(r) = \frac{\chi^{(Q)}(r)}{r}$$

- Equations for the coefficients d_j:

$$\langle\mathcal{A}\Psi u_{\kappa m}|H_{N+1} - E|\phi_{j'}\rangle + \sum_{j}^{m_d} d_j\langle\phi_j|H_{N+1} - E|\phi_{j'}\rangle = 0,\ \ j' = 1,\ldots,m_d,$$

  where $\phi_j = |\gamma_j PJM;N+1\rangle$.
- The two complex scattering amplitudes $f(\vartheta)$ and $g(\vartheta)$ are defined as

$$f(\vartheta) = \frac{1}{2\mathrm{i}k}\sum_l\{(l+1)[\exp(2\mathrm{i}\delta_l^+) - 1] + l[\exp(2\mathrm{i}\delta_l^-) - 1]\}P_l(\cos\vartheta)$$
$$g(\vartheta) = \frac{1}{2k}\sum_l[\exp(2\mathrm{i}\delta_l^-) - \exp(2\mathrm{i}\delta_l^+)]P_l^1(\cos\vartheta)$$

  where ϑ is the scattering angle and P_l and P_l^1 are Legendre polynomial and Legendre associated function, respectively; $\delta_l^{\pm}$ are the relativistic phase shifts, where $+$ refers to the solution with $\kappa = -l-1$ and $-$ to that with $\kappa = l$ (Kessler, 1985).
- The spin polarization for an unpolarized incident beam are given by

$$S(\vartheta) = \frac{i(fg^* - f^*g)}{\sigma(\vartheta)}$$

  where $\sigma(\vartheta) = |f|^2 + |g|^2$ is the differential cross section.

Conclusions

Relativistic multiconfiguration calculations of the differential cross sections and spin polarizations for the elastic scattering of electrons by xenon atoms have been performed using a new method and recently developed computer programs. The results are in good agreement with other available data, both experimental and theoretical. This fact was expected, as the method has some advantages over model-polarization potential, i.e. in taking into account dynamic effects in a precise *ab initio* manner. The method is parameter-free and can be applied to any closed- or open-shell atom. In particular, it should be suitable for heavy atoms, where relativistic effects play an important role.

Differential Cross Sections

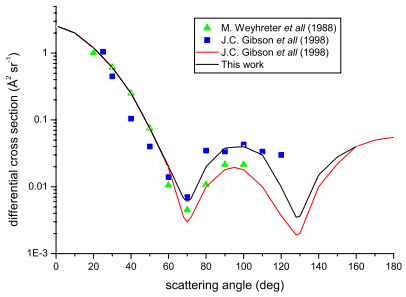

Fig.1. Differential cross section at 0.67 eV against scattering angle.
Squares and triangles, experimental results; full curves, theoretical results.

Spin Polarization

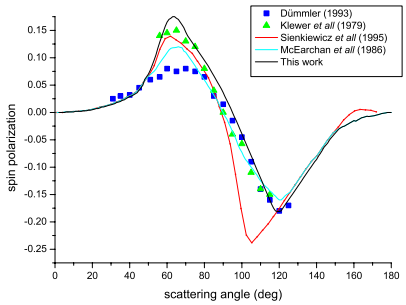

Fig.2. Spin polarization at 10 eV against scattering angle.
Squares and triangles, experimental results; full curves, theoretical results.

All the computations have been performed at the Academic Computer Center in Gdańsk TASK.
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