The relativistic J-matrix method in elastic scattering of slow electrons from Argon atoms

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Theory

SCATTERING EQUATION

Let's start with Dirac equation:

$$\left(H_0-\frac{E}{c\hbar}+\frac{V}{c\hbar}\right)\Psi(r)\equiv\begin{pmatrix}\frac{mc^2-E+V}{c\hbar} & -\frac{d}{dr}+\frac{\kappa}{r}\\ \frac{d}{dr}+\frac{\kappa}{r} & \frac{-mc^2-E+V}{c\hbar}\end{pmatrix}\Psi(r)=\begin{pmatrix}0\\0\end{pmatrix},$$

where $V=V(r)$ is the radial scattering potential, vanishing faster than the Coulomb one, E is the total energy of the projectile. Here, $\Psi=\Psi(r)$ is the relativistic wave function, satisfying the following asymptotic condition:

$$\Psi(r)\xrightarrow{r->\infty}\sin\left(kr-\frac{\pi l}{2}\right)+\tan\delta\cos\left(kr-\frac{\pi l}{2}\right),$$

where δ is the relativistic phase shift, l is the angular momentum of the projectile, $\kappa=-l-1$ or $\kappa=l$, and $k\equiv\sqrt{(E-mc^2)(E+mc^2)}/c\hbar$.

BASIS SET

Let's choose the basis set [1]:

$$\Phi_n^+(r)\equiv\begin{pmatrix}\phi_n^l(\lambda r)\\0\end{pmatrix},$$
$$\Phi_n^-(r)\equiv\begin{pmatrix}0\\\psi_n^l(\lambda r)\end{pmatrix},\qquad \psi_n^l(\lambda r)=\left(\frac{\kappa}{r}+\frac{d}{dr}\right)\phi_n^l(\lambda r).$$

The most popular choice of basis set ϕ_n^l is the complete oscillatory basis set:
$\phi_n^l=r(-1)^n\sqrt{\frac{2n!}{b^3\Gamma(n+l+3/2)}}\left(\frac{r}{b}\right)^l\exp\left(-\frac{r^2}{2b^2}\right)L_n^{(l+1/2)}\left(\frac{r^2}{b^2}\right)$.
Here, $L_n^{(\alpha)}(x)$ are the Laguerre polynomials and b is the oscillator length.
The other popular basis set is the Laguerre basis: $\phi_n^l=(\lambda r)^{l+1}\exp\left(-\frac{\lambda r}{2}\right)L_n^{(2l+1)}(\lambda r)$. In this case, functions ϕ_n^l are biorthonormal, so that $\left\langle\overline{\phi}_m^l\,\middle|\,\phi_n^l\right\rangle\equiv\int_0^\infty\overline{\phi}_m^l(\lambda r)\,\phi_n^l(\lambda r)\,dr=\delta_{mn}$, and λ is the scaling parameter.

JACOBI MATRIX

In such defined bases, the term

$$J_{mn}^{ss'}\equiv\left\langle\Phi_m^s\,\middle|\,\left(H_0-\frac{E}{c\hbar}\right)\Phi_n^s\right\rangle,\quad s,s'=\pm,\quad m,\quad n=0,1,...$$

gives the tridiagonal form (Jacobi matrix).
These so called J-matrix elements $J_{mn}^{ss'}$ can be written as

$$J_{mn}=\begin{pmatrix}-k\epsilon\left\langle\phi_m^l\,\middle|\,\phi_n^l\right\rangle & \left\langle\psi_m^l\,\middle|\,\psi_n^l\right\rangle\\ \left\langle\psi_m^l\,\middle|\,\psi_n^l\right\rangle & -\frac{k}{\epsilon}\left\langle\psi_m^l\,\middle|\,\psi_n^l\right\rangle\end{pmatrix}_{ss'},$$

where $\epsilon\equiv\sqrt{\frac{E-mc^2}{E+mc^2}}$. Now, the J-matrix elements can be easily calculated.

SINE- AND COSINELIKE EXPANSIONS

To assure proper asymptotic behaviour, we introduce sine- and cosine-like solutions of equation:

$$\left(H_0-\frac{E}{c\hbar}\right)\Psi_U=\begin{pmatrix}\Omega_U\overline{\phi}_0^l\\0\end{pmatrix},\quad \Omega_S=0,\quad \Omega_C=-\frac{\epsilon}{s_0^l}.$$

In the above, the indexes U,C corresponds to sine- and cosine-like solutions. The solutions, expanded in the selected basis, are as follows:

$$U(k,r)=\sum_{n=0}^\infty u_n^l(k)\begin{pmatrix}\phi_n^l\\\frac{\epsilon}{\kappa}\psi_n^l\end{pmatrix},\quad U=S,C,\quad u=s,c.$$

Now, the following recursive relations are fulfilled:
$\sum_{n=0}^\infty J_{mn}s_n^l=0$, $\sum_{n=0}^\infty J_{mn}c_n^l=-\frac{k}{2s_0^l}\overline{\phi}_0^l$, $J_{00}s_0^l+J_{01}s_1^l=0, J_{00}c_0^l+J_{01}c_1^l=-\frac{k}{2s_0^l}$ $J_{n,n-1}u_{n-1}^l+J_{n,n}u_n^l+J_{n,n+1}u_{n+1}^l=0; u=s,c; n>1$

POTENTIAL SCATTERING

Let us replace this scattering potential by a truncated potential operator:

$$V_{mn}^N=\begin{pmatrix}\left\langle\phi_m^l\,\middle|\,V/c\hbar\phi_n^l\right\rangle & 0\\ 0 & \left\langle\psi_m^l\,\middle|\,V/c\hbar\psi_n^l\right\rangle\end{pmatrix},m,n=0,1,...N-1$$

Hence, the scattering equation has the following form:

$$\left(H_0-\frac{E}{c\hbar}+V^N\right)\Psi^N(r)\equiv\begin{pmatrix}0\\0\end{pmatrix},\ \text{with expanded solution:}\quad \Psi^N=\sum_{m=0}^{N-1}\begin{pmatrix}d_m^+\phi_m^l\\ d_m^-\frac{\epsilon}{k}\psi_m^l\end{pmatrix}+\sum_{m=N}^\infty\begin{pmatrix}(s_m^++tg\delta_Nc_m^+)\,\phi_m^l\\(s_m^-+tg\delta_Nc_m^-)\,\psi_m^l\end{pmatrix}.$$

In graphical form:

$$\begin{pmatrix}\cdot&\cdot&\cdot&&&&&&&&&&&\cdot&\cdot&\cdot\\ &X&X&X&&&&0&&&&&X&X&X&\\ &&X&X&X&&&&&&X&X&X&&\\ &&&X&X&X&X&X&X&&&X&X&X&&\\ &&&&X&X&X&X&X&&&X&X&X&&\\ &&&&X&X&X&X&X&&X&X&X&&&\\ &&&&X&X&X&X&X&X&X&X&&&&\\ &&&&X&X&X&X&X&X&X&X&&&&0\\ &0&&&&&X&X&X&X&X&X&X&&&\\ &&&&&X&X&X&X&X&X&X&X&&&\\ &&&&X&X&X&&X&X&X&X&X&&&\\ &&&&X&X&X&&X&X&X&X&X&&&\\ &&&X&X&X&&&&X&X&X&&&&\\ &&X&X&X&&&&&&X&X&X&&&\\ &X&X&X&&&&0&&&&&X&X&X&\\ \cdot&\cdot&\cdot&&&&&&&&&&&\cdot&\cdot&\cdot\end{pmatrix}\begin{pmatrix}\cdot\\\cdot\\s_N^++tg\delta_Nc_N^+\\d_{N-1}^+\\\cdot\\\cdot\\d_1^+\\d_0^+\\d_0^-\\d_1^-\\\cdot\\\cdot\\d_{N-1}^-\\s_N^-+tg\delta_Nc_N^-\\\cdot\end{pmatrix}=\begin{pmatrix}0\\0\\0\\0\\0\\0\\0\\0\\0\\0\\0\\0\\0\\0\\0\\0\end{pmatrix}.$$

Equations for $m>N$ are automatically fulfilled, so the following equations remain:

$$\begin{pmatrix}-J_{N,N-1}^{++}c_{N-1}^+ & J_{N,N-1}^{++} & 0 & \cdots & 0 & J_{N,N-1}^{+-} & -J_{N,N-1}^{+-}c_{N-1}^-\\ J_{N-1,N}^{++}c_N^+ & (J+V^N)_{N-1,N-1}^{++} & (J+V^N)_{N-1,N-2}^{++} & \cdots & J_{N-1,N-2}^{+-} & J_{N-1,N-1}^{+-} & J_{N-1,N}^{+-}c_N^-\\ 0 & (J+V^N)_{N-2,N-1}^{++} & (J+V^N)_{N-2,N-2}^{++} & \cdots & J_{N-2,N-2}^{+-} & J_{N-2,N-1}^{+-} & 0\\ \vdots & \vdots & \vdots & \cdots & \vdots & \vdots & \vdots\\ 0 & (J+V^N)_{0,N-1}^{++} & (J+V^N)_{0,N-2}^{++} & \cdots & (J+V^N)_{0,N-2}^{+-} & (J+V^N)_{0,N-1}^{+-} & 0\\ 0 & (J+V^N)_{0,N-1}^{-+} & (J+V^N)_{0,N-2}^{-+} & \cdots & (J+V^N)_{0,N-2}^{--} & (J+V^N)_{0,N-1}^{--} & 0\\ \vdots & \vdots & \vdots & \cdots & \vdots & \vdots & \vdots\\ 0 & J_{N-2,N-2}^{-+} & J_{N-2,N-2}^{-+} & \cdots & (J+V^N)_{N-2,N-2}^{--} & (J+V^N)_{N-2,N-1}^{--} & 0\\ J_{N-1,N}^{-+}c_N^+ & J_{N-1,N-1}^{-+} & J_{N-1,N-2}^{-+} & \cdots & (J+V^N)_{N-1,N-2}^{--} & (J+V^N)_{N-1,N-1}^{--} & J_{N-1,N}^{--}c_N^-\\ -J_{N,N-1}^{-+}c_{N-1}^+ & J_{N,N-1}^{-+} & 0 & \cdots & 0 & J_{N,N-1}^{--} & -J_{N,N-1}^{--}c_{N-1}^-\end{pmatrix}\times\begin{pmatrix}t_N\\d_{N-1}^+\\d_{N-2}^+\\\vdots\\d_0^+\\d_0^-\\\vdots\\d_{N-2}^-\\d_{N-1}^-\\t_N\end{pmatrix}=\begin{pmatrix}J_{N,N-1}^{++}s_{N-1}^+ + J_{N,N-1}^{+-}s_{N-1}^-\\ -J_{N-1,N}^{++}s_N^+ - J_{N-1,N}^{+-}s_N^-\\0\\\vdots\\0\\0\\\vdots\\0\\-J_{N-1,N}^{-+}s_N^+ - J_{N-1,N}^{--}s_N^-\\J_{N,N-1}^{-+}s_{N-1}^+ + J_{N,N-1}^{--}s_{N-1}^-\end{pmatrix}.$$

THE SOLUTION

The tangent of approximated phase shift is given by the formula:

$$\tan\delta_N=-\frac{s_{N-1}^l(k)+\frac{2\epsilon}{k}G_{N-1,N-1}^{++}(E)\,\mathrm{J_{N,N-1}(k)\,s_N^l(k)}}{c_{N-1}^l(k)+\frac{2\epsilon}{k}G_{N-1,N-1}^{++}(E)\,\mathrm{J_{N,N-1}(k)\,c_N^l(k)}},$$

where $G_{mn}^{ss'}(E)=\sum_{p=\pm}\sum_{i=0}^{N-1}c\hbar\frac{\Gamma_{mi}^{sp}\Gamma_{ni}^{s'p}}{E_i^p-E}$, and $\left(\Gamma^\dagger P_N^\dagger\left(H_0+\frac{V}{c\hbar}-\frac{E}{c\hbar}\right)P_N\Gamma\right)_{mn}^{ss'}=\frac{1}{c\hbar}(E_n^s-E)\,\delta_{nm}\delta_{ss'}$.

The elements s_n^l and c_n^l can be found using recursive relations mentioned above [2, 3]. Matrix G can be viewed as the matrix approximating the Green function.
We expect, that $\tan\delta_N\xrightarrow{N->\infty}\tan\delta$ (approximate solution approaches the real value with increasing the basis size). Differential cross section can be then calculated using the following formulas:

$$\sigma(\vartheta)=|f(\vartheta)|^2+|g(\vartheta)|^2, f(\vartheta)=\frac{1}{2ik}\sum_l\{(l+1)[\exp(2i\delta_N^+)-1]+l[\exp(2i\delta_N^+)-1]\}P_l(\cos\vartheta), g(\vartheta)=\frac{1}{2ik}\sum_l[\exp(2i\delta_N^-)-\exp(2i\delta_N^+)]P_l^1(\cos\vartheta)$$

where δ_N^+ corresponds to the solution for $\kappa=l$, and δ_N^- for $\kappa=-l-1$.

Results

OVERVIEW

The most important thing in applications of the J-matrix method to scattering, is to find a good model, properly describing interactions between target and the projectile. Unfortunately, the method itself (in its original form) allows only for specifying the scattering potential only in analytical form. In practice, it means that we need a formula for scattering potential, which, in turn, is used to calculate the potential matrix (by numerical scattering). This, in fact, is rather a significant limitation of the method, because in many cases we have the very accurate target-projectile interactions, but given only in a numerical forms, without any formula. The first, most obvious method to avoid this limitation, could be to use a interpolation over the numerical data, but it could also lead to growing up the numerical error. In this contribution we have obviated this limitation, by using a modified integrating formula, which does not need the integrand in analytical form, thus allowing for using numerical potentials.

THE JMATRIX CODE

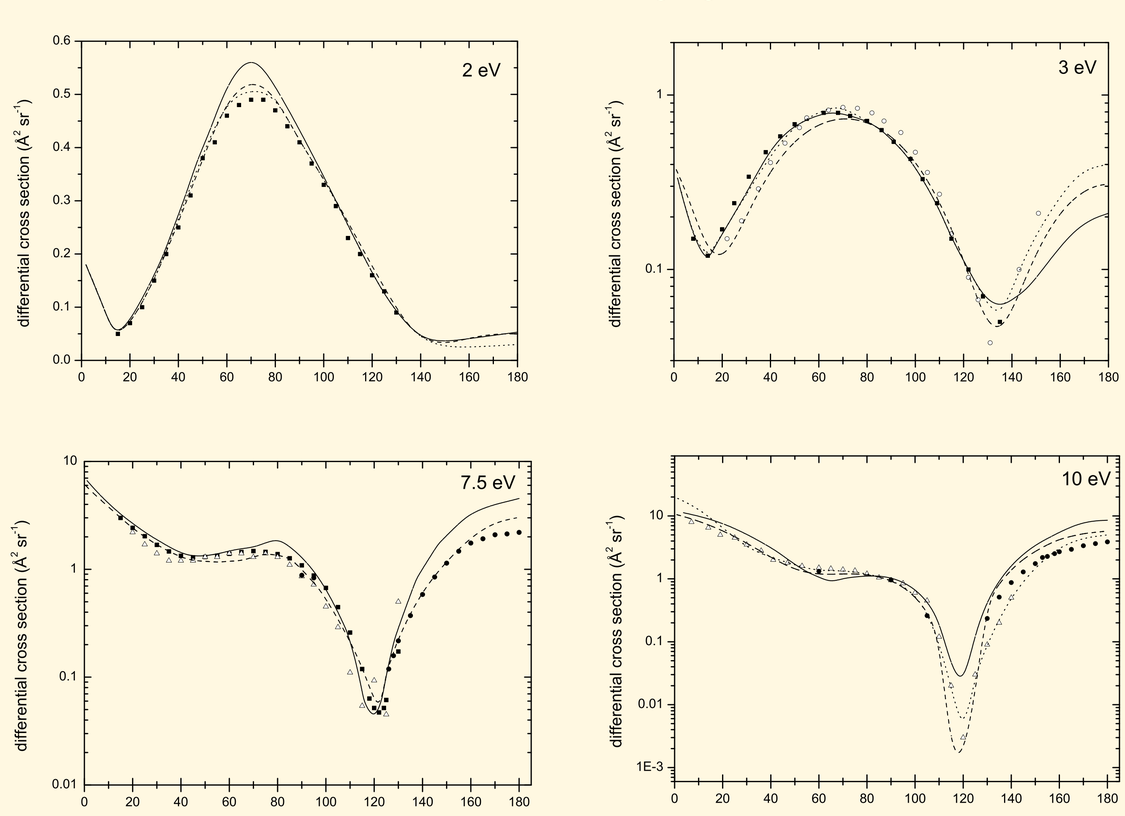
All the J-matrix calculations has been performed by using our own Fortran 95 computer code named JMATRIX, implementing the method. Program allows for relativistic phase shifts calculations for scattering of electrons from several types of potentials: some model potentials given in analytical forms, the approximate atomic potentials, and potentials given in numerical forms. Using this code we can observe convergence of the numerical phase shift together with increasing basis size, then calculating phase shifts for different energies with relatively small computational time.

COMPUTATIONAL PROCEDURE

Although we have announced using the modified relativistic J-matrix method, we have used the regular method (described in the Theory section) in our calculations instead It was because the idea of modifications of the relativistic version of the J-matrix is quite new, and we didn't implemented it yet in the JMATRIX code. We have used the numerical electron-Argon potential, calculated in frames of the Muticonfiguration Dirac-Fock Method using the GRASP92 package [4] using procedure described in [5]. We have used 500 oscillatory basis function to form a basis set, then the matrix potential has been formed. The next step was to calculate phase shifts for selected electron energies. We calculated phase shifts up to $l=10$ and then we used the approximate formula of Ali and Fraser [6], up to $l=50$. Then, differential phase shifts has been calculated.

DIFFERENTIAL CROSS SECTIONS

Relativistic differential cross sections versus scattering angle:



L E G E N D

All graphs:
- solid line: current results

Upper left:
- full squares: Gibson et al (1996; for exact citations of the comparison data, see [5] and references therein)
- dashed line: McEachran and Stauffer (1997)
- dotted line: Syty and Sienkiewicz (1995)

Upper right:
- full squares: Gibson et al (1996)
- empty circles: Williams (1979)
- dashed line: McEachran and Stauffer (1983)
- dotted line: Syty and Sienkiewicz (1995)

Bottom left:
- full squares: Mielewska (2004)
- empty squares: Gibson *et al* (1996)
- empty triangles: Srivastava *et al* (1981)
- dashed line: Syty and Sienkiewicz (1995)

Bottom right:
- full circles: Mielewska (2004)
- empty triangles: Furst *et al* (1989)
- dashed line: Plenkiewicz *et al* (1988)
- dotted line: Syty and Sienkiewicz (1995)

Present work is only a preliminary attempt to use the relativistic J-matrix method to scattering. Current results stay in a good agreement with previous theoretical and experimental data. However, it is clearly visible, that the MCDF calculations [5] are in a much better agreement with experiment at big angles.

References

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