Test of the J-matrix program: electron scattering from the Yukawa potential

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The J-matrix method

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 behavior, 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:
$\sum_{n=0}^{\infty} J_{mn}s_n^l = 0$, $\sum_{n=0}^{\infty} J_{mn}c_n^l = -\frac{k}{2s_0^l}\bar{\varphi}_0^l$, $J_{00}s_0^l + J_{01}s_1^l = 0, J_{00}c_0^l + J_{01}c_1^l = -\frac{k}{2s_0^l}$ $J_{n,n-1}u_{n-1}^l + J_{n,n}u_n^l + J_{n,n+1}u_{n+1}^l = 0; u = s,c; n > 1$

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:

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

In graphical form:

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

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 to the approximated phase shift is given by the formula:

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

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 $\tan\delta_{N,l} \xrightarrow{N->\infty} \tan\delta_l$.

Differential σ_d, total σ_t, spin polarization σ_{sp} and momentum transfer σ_{mt} cross sections:

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

$$\sigma_t(E) = \frac{4\pi}{k^2}\sum_l[(l+1)\sin^2\delta_{N,l}^+ + l\sin^2\delta_{N,l}^-], \quad \sigma_{sp}(\vartheta) = \frac{i(f(\vartheta)g^*(\vartheta) - f^*(\vartheta)g(\vartheta))}{\sigma_d(\vartheta)}, \quad \sigma_{mt}(E) = \frac{4\pi}{k^2}\sum_l\Big[\frac{(l+1)(l+2)}{2l+3}\sin^2(\delta_{N,l}^+ - \delta_{N,l+1}^+) + (...)\Big],$$

where $\delta_{N,l}^-$ corresponds to the solution for $\kappa = l$, and $\delta_{N,l}^+$ for $\kappa = -l-1$.

Scattering from a Yukawa potential

To illustrate the application of the J-matrix method in scattering, we consider the electron scattering from the screened Yukawa potential, in the presence of a high-frequency laser field.

THE HIGH-FREQUENCY CLASSICAL APPROXIMATION

Let's assume, that the monochromatic, electromagnetic field of the constant intensity, is linearly polarized in the z direction [4]. The vector potential is then:

$$A(t) = A_0\cos(\omega t + \phi).$$

The Hamiltonian is given by:

$$H = \frac{p^2}{2m} + V(r + \alpha_0\sin(\omega t + \phi)),$$

where $\alpha_0 = \frac{eA_0}{m\omega} = \frac{\sqrt{I}}{\omega^2}$ is the amplitude of the oscillations (of the frequency ω) of a free electron of the mass m, in the external field of the intensity I. Now, let's write the leading two terms of the Fourier expansion of the above time-dependent Hamiltionian:

$$V(r,t,\alpha_0,\omega) = V_0(r,\alpha_0) + V_1(r,\alpha_0)\sin(\omega t).$$

The time-averaged, time-independent part of the expansion, V_0, is called the dressed potential. In the present calculations, we neglect the time-dependent, second term of the expansion.

THE DRESSED YUKAWA POTENTIAL

Yukawa potential is, in general, the kind of potential giving rise to the strong force, acting between nucleons, and is due to to virtual meson exchange [5]. Scattering from Yukawa potential can be also seen as the model of the electron-atom interaction and exhibits the Coulomb singularity [4]. If we consider the Yukawa potential in the form

$$V(r) = -\frac{e^{-\mu r}}{r},$$

then the dressed Yukawa potential can be written as

$$V_0(r,\alpha_0) = \frac{1}{\pi}\int_{-\frac{\pi}{2}}^{\frac{\pi}{2}} V(|r + \alpha_0\sin u|)du.$$

The exponential behavior of $V(r)$ makes it a short-range potential.

NUMERICAL PROCEDURE

First, the dressed Yukawa potential has been calculated, by the numerical integration. Then, the regular, relativistic J-matrix method has been used to solve the scattering problem. To expand the solution, 1000 oscillatory basis function have been used, then the potential and Jacobi matrices have been formed. The next step was to calculate phase shifts for selected electron energies, up to $l = 20$. Then, the appropriate cross sections have been calculated.

RESULTS

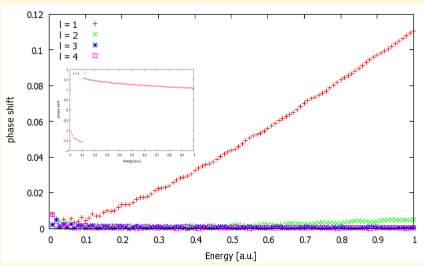

Figure 1. Phase shifts versus energy of the projectile. For clarity, phase shifts for different $\kappa = l$, $\kappa = -l-1$ and $l > 4$ has been omitted, and the graph for $l = 0$ has been plotted separately. The irregularities originates from integrating error in calculating the dressed Yukawa potential, and integrating error in calculating the potential matrix. In all calculations $\alpha_0 = 0.5$ and $\mu = 0.5$ were used.

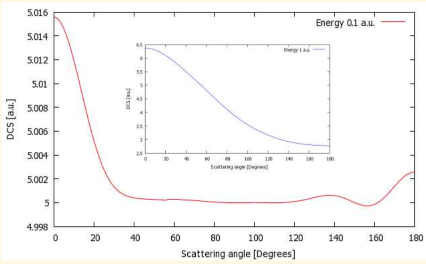

Figure 2. Differential cross section $\sigma_d(\vartheta)$ versus the scattering angle, calculated for electron energy $E = 0.1$a.u. (the main graph) and $E = 1$a.u. (the inner graph).

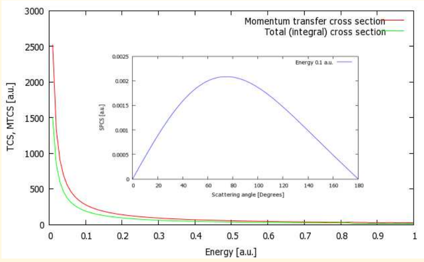

Figure 3. Total (elastic) cross section $\sigma_t(E)$ and momentum transfer cross section $\sigma_{mt}(E)$ (the main graph). Spin polarization cross section $\sigma_{sp}(\vartheta)$ (the inner graph; $E = 0.1$a.u).

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