The relativistic J-matrix method in scattering of electrons from model potentials and small 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:

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

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]:

$$\Phi_n^+(r)\equiv\begin{pmatrix}\phi_n^l(\lambda r)\\0\end{pmatrix},$$

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

We have two choices of the function ϕ_n^l: Laguerre basis, $\phi_n^l=(\lambda r)^{l+1}\exp\left(-\frac{\lambda r}{2}\right)L_n^{(2l+1)}(\lambda r)$, and the Gaussian basis, $\phi_n^l=(\lambda r)^{l+1}\exp\left(-\frac{\lambda^2r^2}{2}\right)L_n^{(l+1/2)}(\lambda^2r^2)$ - so we obtain two different basis sets. Here, $L_n^{(\alpha)}(x)$ are the Laguerre polynomials, λ is the scaling parameter. Functions ϕ_n^l are biorthonormal: $\left\langle\overline{\phi}_m^l\,\middle|\,\phi_n^l\right\rangle\equiv\int_0^\infty\overline{\phi}_m^l(\lambda r)\,\phi_n^l(\lambda r)\,dr=\delta_{mn}$. However, knowledge of the biorthonormal elements $\overline{\phi}_m^l$ is not necessary.

JACOBI MATRIX

In such defined bases, the term

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

gives the tridiagonal form.
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 $\epsilon\equiv\sqrt{\frac{E-mc^2}{E+mc^2}}$. Let's also introduce the non-relativistic J-matrix elements (but taken in the relativistic point k), simply related to the above integrals:

$$\mathrm{J}_{mn}=\frac{1}{2}\left\langle\psi_m^l\,\middle|\,\psi_n^l\right\rangle-\frac{k^2}{2}\left\langle\phi_m^l\,\middle|\,\phi_n^l\right\rangle.$$

SINE- AND COSINELIKE EXPANSIONS

To assure proper asymptotic behaviour, we introduce sine- and cosinelike 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 cosinelike 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:
$\sum_{n=0}^{\infty}J_{mn}s_n^l=0$, $\sum_{n=0}^{\infty}J_{mn}c_n^l=-\frac{k\epsilon}{2s_0^l}\overline{\phi}_m^l$, $J_{00}s_0^l+J_{01}s_1^l=0, J_{00}c_0^l+J_{01}c_1^l=-\frac{k\epsilon}{2s_0^l}$ $J_{n,n-1}u_{n-1}^l+J_{n,n}u_n^l+J_{n,n+1}u_{n+1}^l=0; u=s,c; n>1$

POTENTIAL SCATTERING

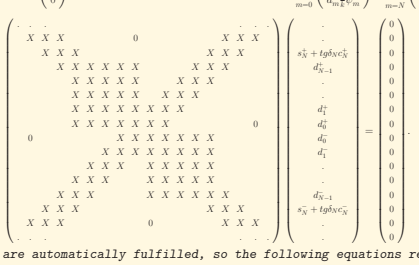
Let us replace this scattering potential by a truncated potential operator:

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

Hence, the scattering equation has the following form:

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

In graphical form:



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:

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

where $G_{mm'}^{ss'}(E)=\sum_{p=\pm}\sum_{i=0}^{N-1}c\hbar\frac{\left\langle mp\right|\left.ip'\right\rangle}{E_i^p-E}$, and $\left(\Gamma^\dagger P_N^\dagger\left(H_0+\frac{V}{c\hbar}-\frac{E}{c\hbar}\right)P_N\Gamma\right)_{mn}^{ss'}=\frac{1}{c\hbar}\left(E_n^s-E\right)\delta_{mn}\delta_{ss'}$.

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.

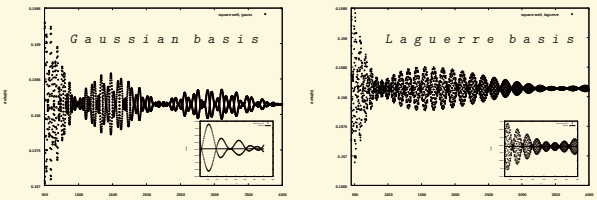
We expect, that $\tan\delta_N\xrightarrow{N\to\infty}\tan\delta$ (approximate solution approaches the real value with increasing the basis size).

Results

We have written the computer code JMATRIX implementing the method, and performed relativistic phase shifts calculations for scattering of electrons from several types of potentials: some model potentials given in analytical forms, and the approximate atomic potentials. In all cases and both bases, we observe convergence of the numerical phase shift together with increasing basis size. Moreover, the method allows for calculating phase shifts for different energies with relatively small computational time.

SQUARE-WELL

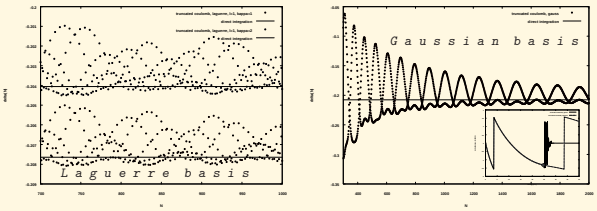
$$V(r)=\begin{cases}0 & \text{for}\quad r\in(0,a)\\ V_0 & \text{for}\quad r\in[a,b)\\ 0 & \text{for}\quad r\in[b,\infty)\end{cases},a=0.8au,b=1au,V_0=-1au,E=3au,l=1,\kappa=1$$



Relativistic phase shifts versus basis size. Comparison with the analytical result [4].

TRUNCATED COULOMB

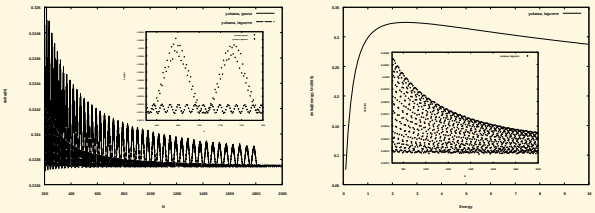
$$V(r)=\begin{cases}\frac{-Z\epsilon^2}{r}, r<r_0\\ 0, r\geq r_0\end{cases},Z=30,r0=1au,E=3au,l=1,\kappa=1,-2$$



Relativistic phase shifts compared to result obtained using direct integration [5]. Small graph: phase shift as function of the projectile energy. Clearly visble defect in the gaussian basis at $E\approx25au$.

YUKAWA POTENTIAL

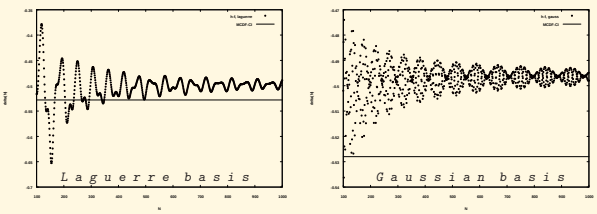
$$V(r)=\frac{-g^2\exp(-mr)}{r},g=1,m=1,E=3au,l=1,\kappa=1$$



Relativistic phase shifts versus basis size, both bases (left graph and small graphs). Right graph: phase shift as function of the projectile energy.

ATOMIC POTENTIAL - ARGON

$$V(r)=\frac{-Z\epsilon^2}{r}\left(\sum_{j=1}^{2}a_j\exp(-b_jr)+r\sum_{j=1}^{n}c_j\exp(-d_jr)\right),\ \text{parametres as given in [6]}$$



Relativistic phase shifts as function of the basis size, compared to result obtained using the MCDF-CI method [7]. The applied potential is rather rough estimation of the real potential, thus the results vary from each other by about 10%. We work on applying much more accurate atomic potentials to the code, i.e. taken from the GRASP92 package [8].

References

[1] P. Horodecki, Phys. Rev. A 62, 052716 (2000)
[2] E. Heller, H. Yamani, Phys. Rev. A 9, 1201 (1974)
[3] H. Yamani, L. Fishman, J. Math. Phys. 16, 410 (1975)
[4] P. Syty, TASK Quarterly 3 No. 3, 269 (1999)
[5] M. Krośnicki, M.Sc. thesis, Gdańsk University of Technology (1998)
[6] T.G. Strand, R.A. Bonham, J. Chem. Phys. 40 1686 (1964)
[7] P. Syty, J.E. Sienkiewicz, J. Phys. B 38, 2859 (2005)
[8] F.A. Parpia, C. Froese Fischer, I.P. Grant, Comput. Phys. Commun. 94, 249 (1996)