Relativistic Corrections to Electronic Scattering Lengths. Results for Strontium.

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Definition

Scattering length is a parameter used to describe low-energy electron-atom collisions. It is defined as the radius of a rigid sphere in the zero-energy total cross-section. The sign of a scattering length represents the type of interaction: positive for repulsion and negative for attraction.

Polarisation potential

$$E = \frac{1}{2}\alpha_d \vec{\mathbf{E}}^2$$

$$V(r) = -\frac{1}{2}\frac{\alpha_d}{r^4} = -\frac{1}{2}\frac{\beta^2}{r^4}$$

$$\vec{\mathbf{E}} = \frac{e\vec{\mathbf{r}}}{\sqrt{(r^3 + r_0^3)^2}},$$

$$V_{pol}(r) = -\frac{1}{2}\frac{\alpha_d r^2}{(r^3 + r_0^3)^2}$$

$$V_{pol}(r) = -\frac{1}{2}\frac{\alpha_d r^2}{(r^3 + r_0^3)^2} - \frac{1}{2}\frac{\alpha_q^{'} r^4}{(r^5 + r_0^5)^2}$$

Parameter β is often called characteristic quantum length.

Dirac's equation - zero energy with polarisation

$$\left(\frac{\mathrm{d}}{\mathrm{d}r}+\frac{\kappa}{r}\right)P_\kappa(r)=\left(\frac{2}{\alpha}+\frac{\alpha\beta^2}{2r^4}\right)Q_\kappa(r)$$

$$\left(\frac{\mathrm{d}}{\mathrm{d}r}-\frac{\kappa}{r}\right)Q_\kappa(r)=-\frac{\alpha\beta^2}{2r^4}P_\kappa(r)$$

$$\frac{\mathrm{d}^2P(r)}{\mathrm{d}r^2}+\frac{1}{r}\frac{4\alpha^2\beta^2}{2r^4+\alpha^2\beta^2}\frac{\mathrm{d}P(r)}{\mathrm{d}r}-\frac{1}{r^2}\frac{4\alpha^2\beta^2}{2r^4+\alpha^2\beta^2}P(r)=\left(-\frac{\beta^2}{r^4}-\frac{\alpha^2\beta^4}{4r^8}\right)P(r)$$

$$\frac{\mathrm{d}^2Q(r)}{\mathrm{d}r^2}+\frac{4}{r}\frac{\mathrm{d}Q(r)}{\mathrm{d}r}+\frac{2}{r^2}Q(r)=\left(-\frac{\beta^2}{r^4}-\frac{\alpha^2\beta^4}{4r^8}\right)Q(r)$$

$$
\begin{aligned}
Q(r) &= \frac{\alpha^2}{4}\Big(\frac{a}{r} + \frac{\beta^2}{r^2} - \frac{\beta^2}{2!}\frac{a}{r^3} - \frac{\beta^4}{3!}\frac{1}{r^4} + \frac{\beta^4}{4!}\frac{a}{r^5} \\
&\quad + \frac{\beta^6}{6!}\frac{1}{r^6} - \frac{\beta^6}{6!}\frac{a}{r^7} - \frac{4!\cdot\frac{\alpha^2\beta^2}{4}}{6!}\frac{a}{r^7} + \dots\Big) \\
&= \frac{\alpha^2}{4}\frac{a}{r}\left(1 - \frac{\beta^2}{2!}\frac{1}{r^2} + \frac{\beta^4}{4!}\frac{1}{r^4} - \frac{\beta^6}{6!}\frac{1}{r^6} + \dots\right) \\
&\quad + \frac{\alpha^2}{4}\frac{\beta}{r}\left(\frac{\beta}{r} - \frac{\beta^3}{3!}\frac{1}{r^3} + \frac{\beta^5}{5!}\frac{1}{r^5} - \dots\right) - \frac{4!\cdot\frac{\alpha^2\beta^2}{4}}{6!}\frac{a}{r^7}\dots \\
Q(r) &= \frac{\alpha^2}{4}\frac{a}{r}\cos\left(\frac{\beta}{r}\right) + \frac{\alpha^2}{4}\frac{\beta}{r}\sin\left(\frac{\beta}{r}\right) + \alpha^4 O\left(\frac{1}{r^7}\right)
\end{aligned}
$$

$$
\begin{aligned}
P(r) &= r - a - \frac{\beta^2}{2}\frac{1}{r} + a\frac{\beta^2}{3!}\frac{1}{r^2} + \frac{\beta^4}{4!}\frac{1}{r^3} - a\left(\frac{\beta^4}{5!} + \frac{4!\cdot\frac{\alpha^2\beta^2}{4}}{5!}\right)\frac{1}{r^4} + \dots \\
&= r\left(1 - \frac{\beta^2}{2}\frac{1}{r^2} + \frac{\beta^4}{4!}\frac{1}{r^4} - \dots\right) - \frac{ar}{\beta}\left(\frac{\beta}{r} - \frac{\beta^3}{3!}\frac{1}{r^3} + \frac{\beta^5}{5!}\frac{1}{r^5} - \dots\right) \\
&- a\frac{4!\cdot\frac{\alpha^2\beta^2}{4}}{5!}A\frac{1}{r^4} + \dots \\
&= r\cos\left(\frac{\beta}{r}\right) - \frac{ar}{\beta}\sin\left(\frac{\beta}{r}\right) + O\left(\frac{1}{r^4}\right) \\
P(r) &= \frac{r}{a}\cos\left(\frac{\beta}{r}\right) - \frac{r}{\beta}\sin\left(\frac{\beta}{r}\right) + \alpha^2 O\left(\frac{1}{r^4}\right)
\end{aligned}
$$

Steps to check

1. Check whether the solution tends to straight line
2. Check whether adding additional coefficients makes better results
3. Check whether we can get back parameter β
4. Check the correctness of a formula with sine and cosine
5. Check whether we can spot the difference between non-relativistic and relativistic equations

Strontium

Some information about strontium:

- Has closed-subshell structure
- $\langle r \rangle = 4.55369$ a.u.
- $\alpha_d = 197.2$ (Schwerdtfeger, P. and Nagle, J. K. 2018)
- $\beta = 14.04279$ ($\beta^2 = \alpha_d$)
- Known scattering lengths: experimental $a = -12.5$ a.u, (Giannakeas, P. and Eiles, Matthew T. and Robicheaux, F. and Rost, Jan M. 2020), $a = -13.2$ a.u (De Salvo 2015) theoretical $a = -18$a.u (Bartschatt, Sadeghpour 2003)

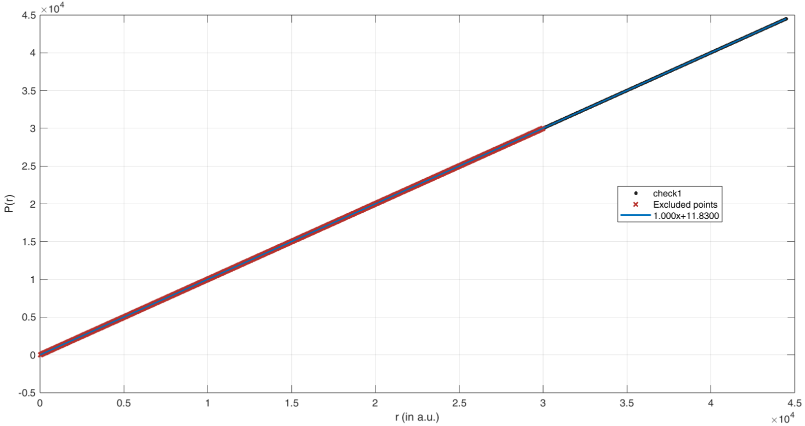


Figure: Claim: Is the straight line approximation correct? Approximation: $P(r) = 1.000r + 11.8300 \rightarrow a = -11.8300$

Test 2

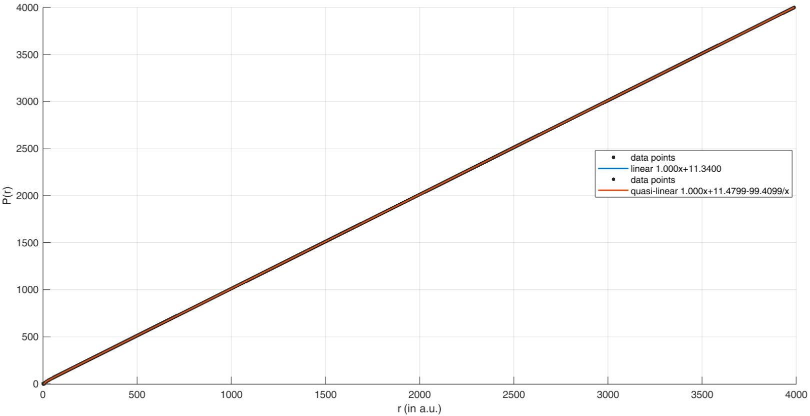
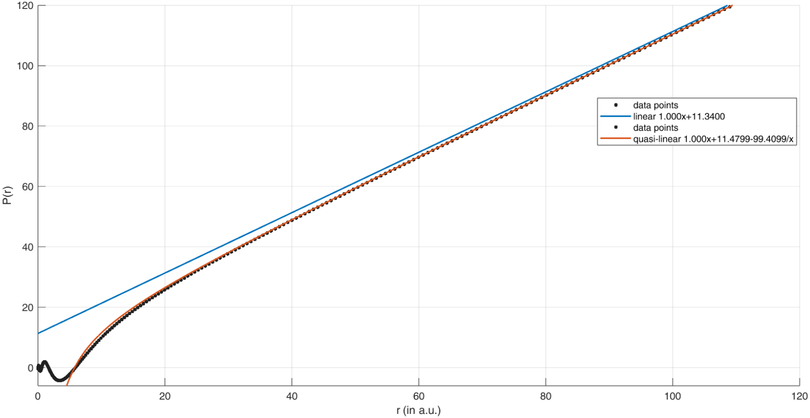


Figure: Claim: Is the longer approximation better? Approximations: $P(r) = 1.000r + 11.3400$ and $P(r) = 1.000r + 11.4799 - 99.4099/r$



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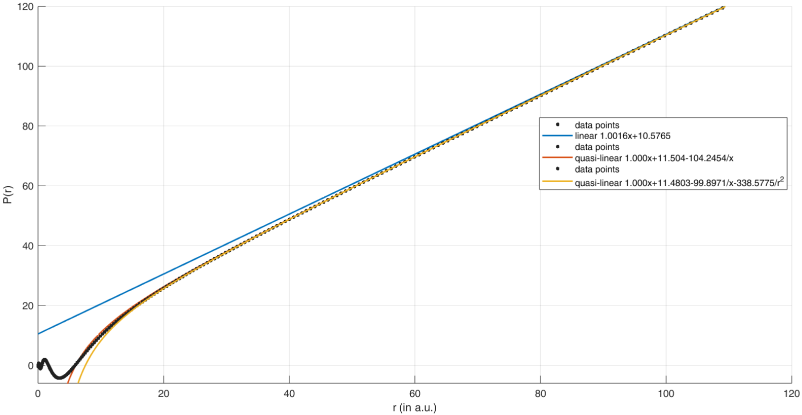

Figure: Claim: Is the longer approximation better? Approximations: $P(r) = 1.0016r + 10.5765$, $P(r) = 1.000r + 11.504 - 104.2454/r$ and $P(r) = 1.000r + 11.4803 - 99.8971/r - 338.5775/r^2$

We know that the coefficient next to r^{-1} is equal to $\frac{-\beta^2}{2}$. From the first approximation we get $\frac{-\beta^2}{2} = -99.4099 \rightarrow \alpha_d = \beta^2 = 198.8198$
From the second approximation
$-\frac{\beta^2}{2} = -99.8971 \rightarrow \alpha_d = \beta^2 = 199.7942$. To recall, in the code we have put $\alpha_d = \beta^2 = 197.2$

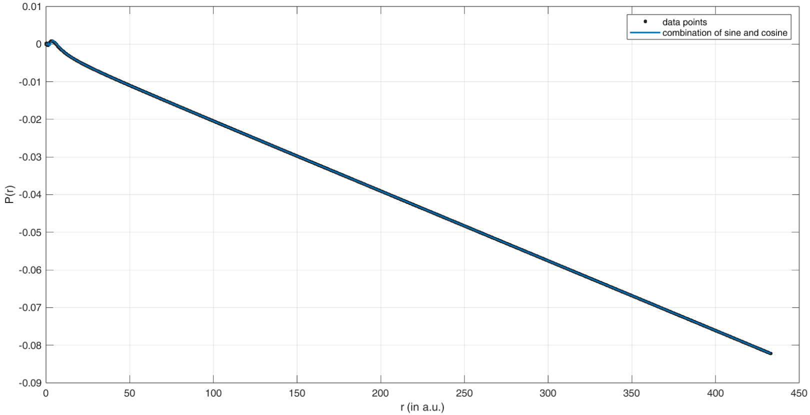

Figure: Claim: Is the sine-cosine approximation better?

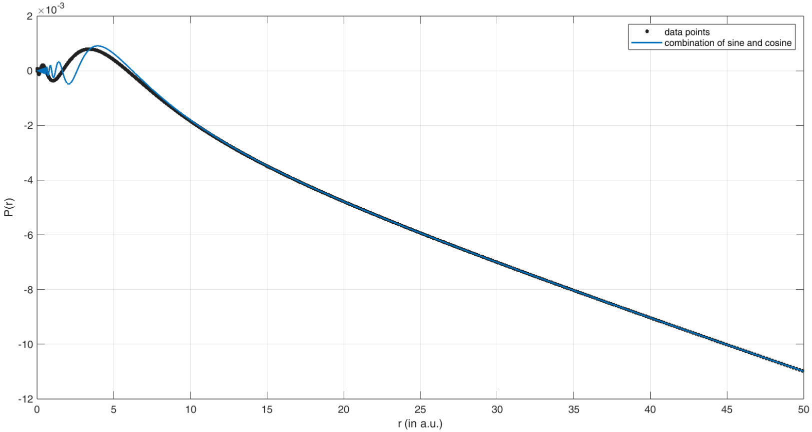

Figure: Claim: Is the sine-cosine approximation better? For this graph we have $P(r) = N(\frac{r}{a}\cos\frac{\beta}{r} - \frac{r}{\beta}\sin\frac{\beta}{r})$ with $a = -11.4751$ a.u and $\beta = 14.0358$.

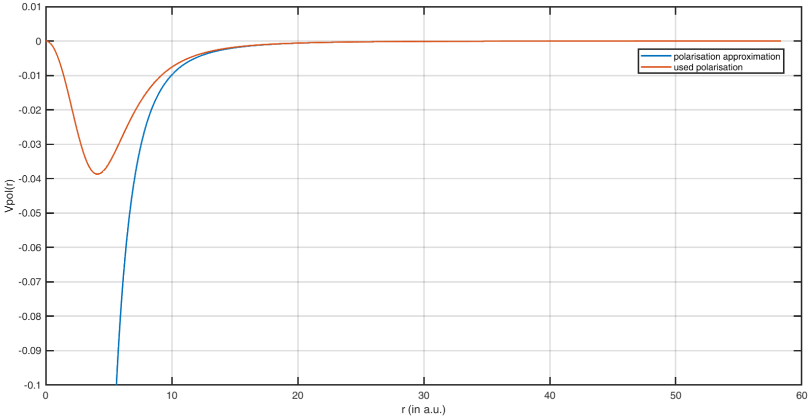

Figure: Comparison between model polarisation potential and potential used in calculations.

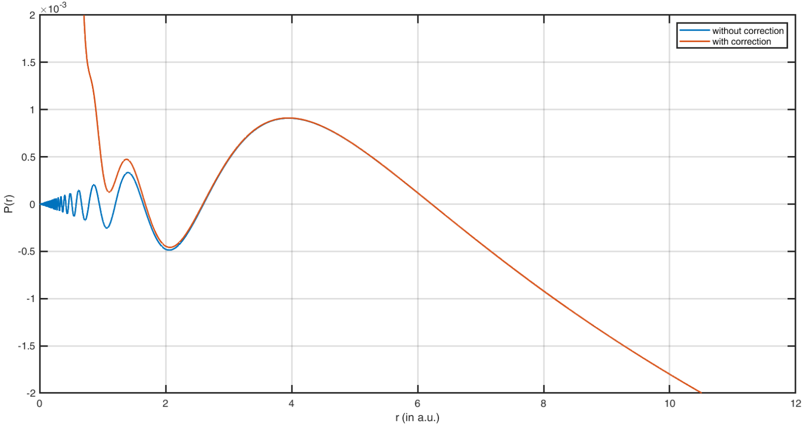

Figure: Comparison between the sine-cosine result with and without relativistic correction.

The end

Thank you for your attention. We will work more on the continuum solutions to Dirac equations.