Summary and collected results

Alessandro Miccichè

August 2025

The project reproduces part of the work in [1].
I. We start from the Coulombic potential (in atomic units and energy expressed in Rydberg):

$$V_C(r) = -2\frac{Z}{r} \tag{1}$$

and through the function `solve_schr` we solve numerically the Schrödinger equation, employing the Numerov's method with a logarithmic grid [1]. We have followed Chapters 1 and 2 of [2], and the code is based on `hydrogen_radial.c` therein. For $l = 0$, we compute:

- eigenfunctions χ_{0n} and eigenvalues E_n up to an arbitrary n_{max} (in the discrete spectrum);
- phase shifts $\delta(E_n)$ at r_{ph}.

Fig. 1 shows the results for the relative error between the analytical and numerical results of the energy levels of an hydrogenlike atom with atomic number $Z = 1$.

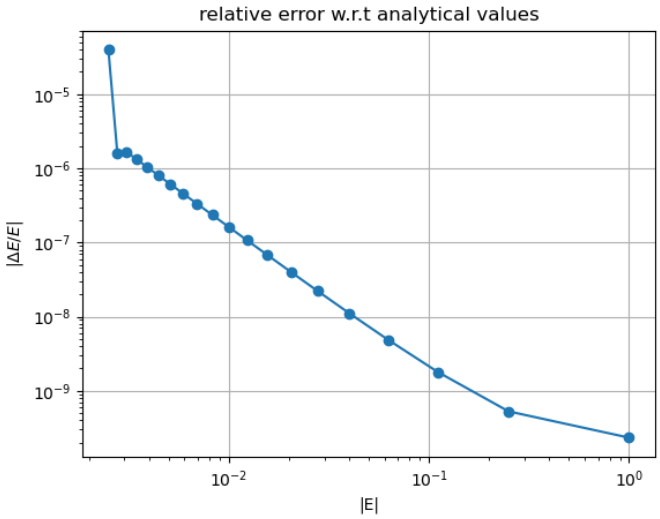

Figure 1: Relative error of the numerical results for the Coulombic energy eigenvalues with respect to the analytical values.

II. Next, we add a short range potential to the Coulombic one. Following Exercise 2.3.3 in [2], we add a Yukawa-type potential:

$$V_{true}(r) = V_C(r) + V_s(r) = V_C(r) - 2Z\frac{e^{-br}}{r} \tag{2}$$

[1] The grid does not contain $r = 0$. It starts from a minimal value $r_{min} \neq 0$. This automatically regulates the singularity in $r = 0$.

being the true potential defining the theory whose low-energy limit we want to study [2]. We compute the same quantities. These will be our reference results.

III. The simplest and less precise approximation is to use first order perturbation theory to compute energy eigenvalues. The short-range potential V_s is approximated by a delta function. At first order, the eigenvalues are

$$E_n = E_{C\,n} + k\frac{\delta_{l\,0}}{\sqrt{\pi}n^3} = -\frac{1}{n^2} + k\frac{\delta_{l\,0}}{\sqrt{\pi}n^3} \tag{3}$$

We fit this expression to our lowest energy data (in absolute value) $E_{n_{max}}$ to find k.

As we shall see, our V_s is not a small perturbation and the first order corrections do not provide an accurate approximation, especially for energy levels with small n. The second order corrections are infinite.

IV. We want to model the low energy behaviour of the true theory through an effective theory, i.e. through an effective potential. The low-energy behaviour of the theory is independent of the details of the high energy dynamics: we can design the effective short potential in order to fit the low energy data generated with the true potential.

Being known the long range behaviour (Coulomb), we mimic the effects of the true short-distance structure by adding local correction terms. Taylor expanding the momentum space potential V_s near 0, and Fourier transforming the first terms, gives correction terms as a polynomial in the momentum operator ∇/i multiplied by a delta function. We introduce an ultraviolet cut-off to avoid infinities and smear the delta function:

$$\delta_a^3(r) = \frac{e^{-r^2/\sqrt{2}a^2}}{(2\pi)^{3/2}a^3} \tag{4}$$

and the effective potential reads:

$$V_{eff}(r) = V_C(r) + c\,a^2\delta_a^3(r) + d_1\,a^4\,\nabla^2\delta_a^3(r) + O(a^6) \tag{5}$$

with c, d_1 dimensionless coupling constants to be tuned in order to reproduce the low energy data. The cut-off distance a sets the range of the effective short potential and the cut-off in momentum space $\Lambda = 1/a$.

Choosing $b = 1$ in (2), the characteristic range of V_s is ≈ 1 . For the cut-off distance, we choose the following values $a = \{0.1, 1, 3, 10\}$. For each of them, we fit the phase shift for $n = n_{max}$ of the true theory with the corresponding phase shift generated by the effective theory, in order to find the values of the couplings c, d_1 for the a^4-theory, and c for the a^2-theory ($d_1 = 0$). This is done using the optimization algorithm `differential_evolution` of the Scipy library [3].

Having found the couplings in the a^4- and a^2-theory, for each a, we compute eigenfunctions, eigenvalues and phase shifts as usual. Below, we show the results for eigenvalues and phase shifts.

[2] To include the effects of the short range potential in the numerical computation, it is necessary that its range, $1/b$, is much bigger than the coordinates of the first grid point r_{min}.

[3] It searches for a global minimum of the squared difference between phase shifts, for values of the couplings in a given interval. If for some values of c and d_1, the function `solve_schr` does not convergence, the optimization algorithm discards these values.

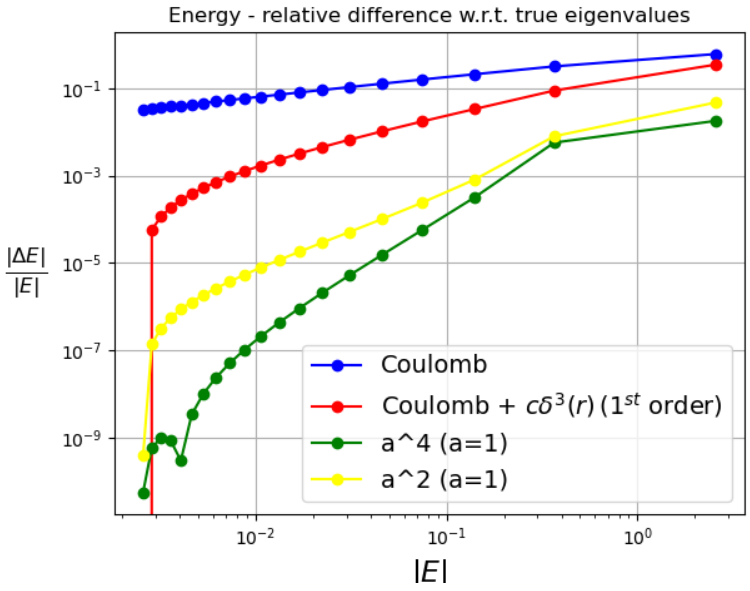

Figure 2: Relative error of the energy levels compared to the true theory

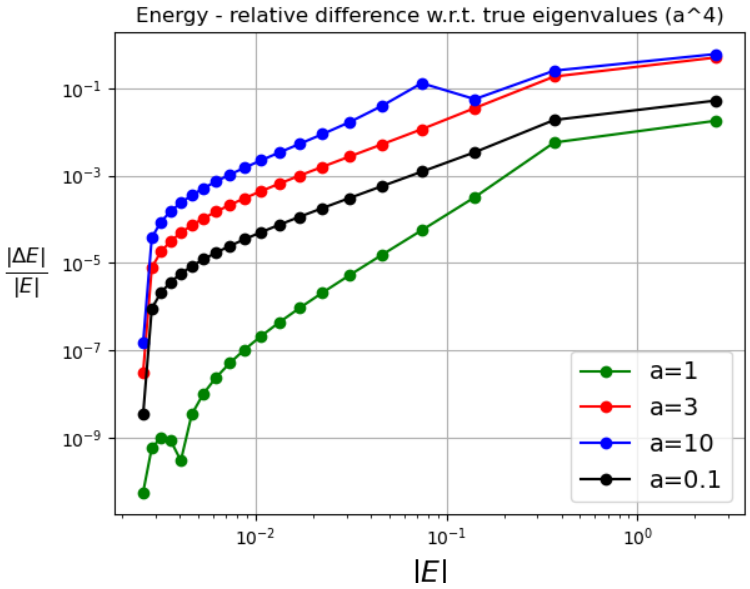

Figure 3: a^4- theory: relative error of the energy levels compared to the true theory.

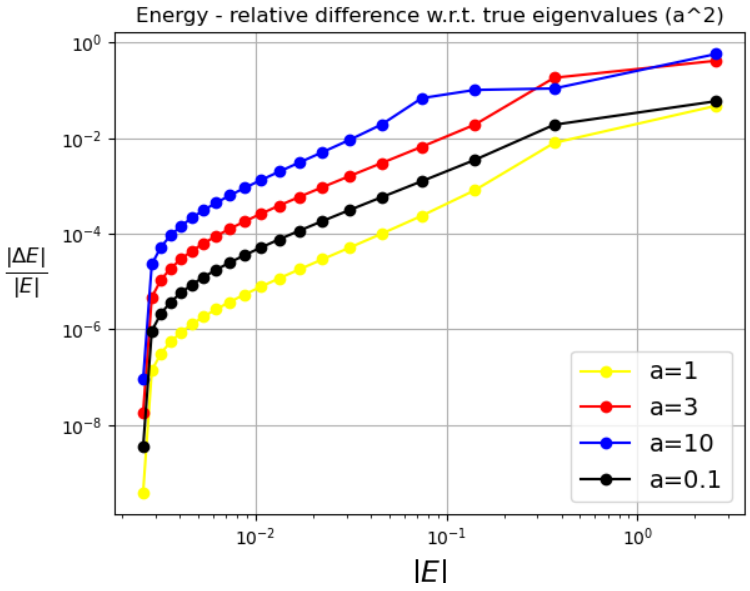

Figure 4: a^2- theory: relative error of the energy levels compared to the true theory.

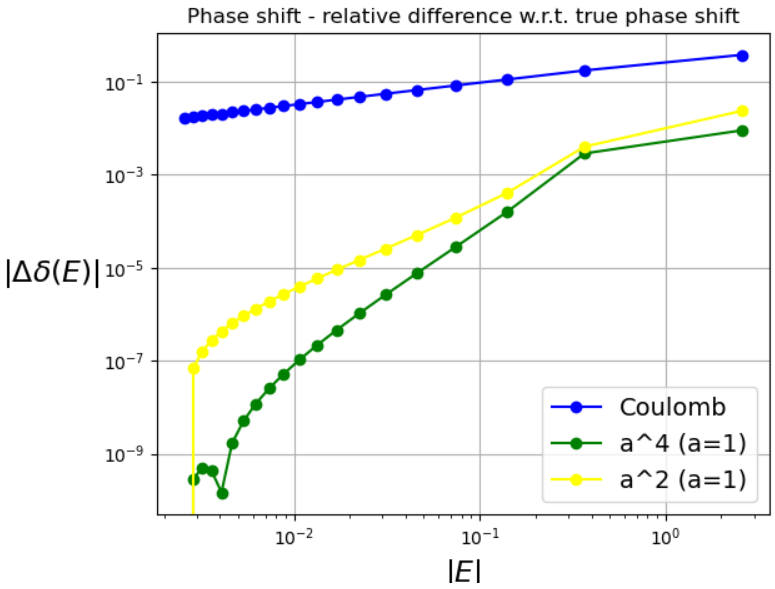

Figure 5: Relative error of the phase shifts (evaluated at $r_{ph} = 800$) compared to the true theory.

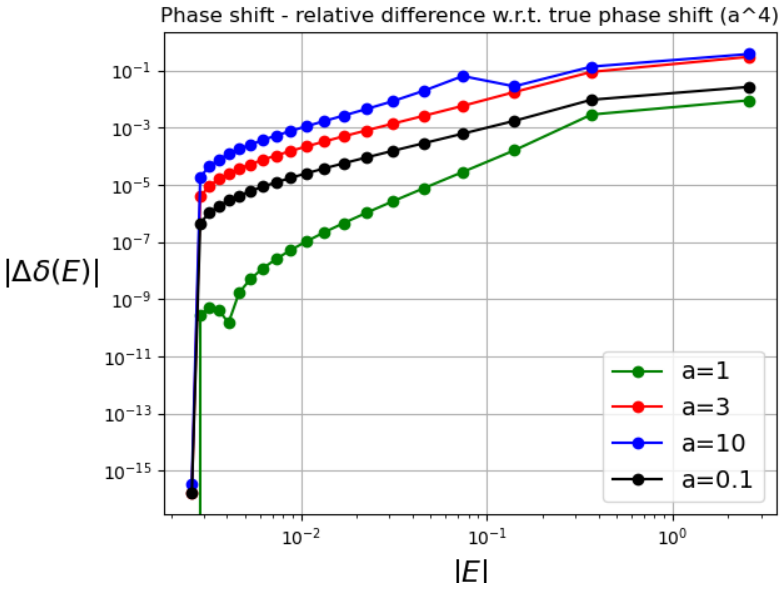

Figure 6: a^4- theory: relative error of the phase shifts (evaluated at $r_{ph} = 800$) compared to the true theory.

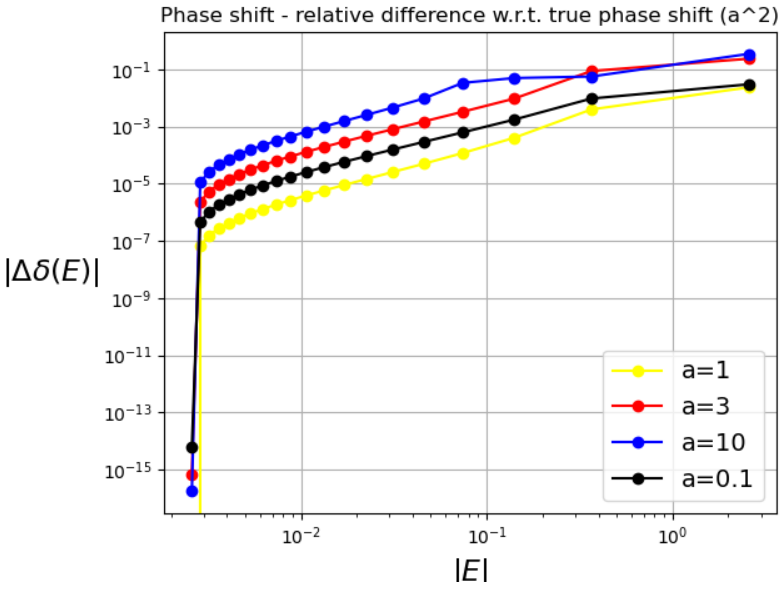

Figure 7: a^2- theory: relative error of the phase shifts (evaluated at $r_{ph} = 800$) compared to the true theory.

References

[1] G. P. Lepage *How to Renormalize The Schrödinger Equation*, 8th Jorge Andre Swieca Summer School on Nuclear Physics, 1997. `https://arxiv.org/abs/nucl-th/9706029`

[2] P. Giannozzi *Numerical Methods in Quantum Mechanics*, Lecture notes.