Numerical Methods in Quantum Mechanics

Accuracy of Numerov Integration Algorithm

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1 Introduction

The aim of this report is to define and study the global error in the famous algorithm by Numerov: a useful tool for solving numerically particular differential equations. The problem will be developed by improving the existing code `harmonic1.f90` to provide a visual demonstration via `gnuplot` of the dependence of the global error from the step chosen for the Numerov's grid, and how it behaves in different situations.
In this report the one-dimensional Scrödinger equation for the harmonic oscillator with constant K will be solved, so the starting point is the canonical form:

$$\frac{d^2\psi(x)}{dx^2} = -\frac{2m}{\hbar^2}\left(E - \frac{1}{2}Kx^2\right)\psi(x) \tag{1}$$

From this, the discrete eigenvalues E_n and the eigenfunctions $\psi_n(x)$ will be calculated and compared with the well-known analytical results to study the implementation's numerical accuracy.

2 Numerov's Algorithm

The Numerov Algorithm is used form the integration of second order differential equations in the form:

$$\frac{d^2y}{dx^2} = -g(x)y(x) + s(x) \tag{2}$$

The known functions $f(x)$ and $g(x)$ are discretized on a set of equispaced x_i obtained by fractioning in N sections Δx the interval $[-x_{max}, +x_{max}]$. Then the $y(x)$ function is expanded around x_n up to the fifth order, and after some manipulations and a change of notation ($y_n'' \longrightarrow z_n$), the recursive *Numerov's Formula* is obtained:

$$y_{n+1}\left[1 + g_{n+1}\frac{(\Delta x)^2}{12}\right] = 2y_n\left(1 - 5g_n\frac{(\Delta x)^2}{12}\right)$$

$$-y_{n-1}\left(1 + g_{n-1}\frac{(\Delta x)^2}{12}\right) + (s_{n+1} + 10s_n + s_{n-1})\frac{(\Delta x)^2}{12} + O(\Delta x^6) \tag{3}$$

The equation leads us to the discrete solution $y(x_{i=1,\dots,N})$; the only condition is the knowledge of the first two steps y_0 and y_1 to start the recurrency.

3 Numerov for the Harmonic Potential

To make use of Numerov on the harmonic oscillator, the Schrödinger equation is manipulated to contain dimensionless units, more convenient in the code drafting. To do so, an adimensional variable χ proportional to the length, and an adimensional energy ε are defined:

$$\varepsilon = \frac{E}{\hbar\omega} \qquad \xi = \sqrt{\frac{m\omega}{\hbar}}x \tag{4}$$

In this formulation, $x \equiv \lambda\xi$, and the following condition is imposed: $1 = m\ K\ \lambda^4\ \hbar^2$.
Substituting this new variables to the previous ones in equation (1), we obtain the new Schrödinger equation:

$$\frac{d^2\psi}{d\xi^2} = -2\left(\varepsilon - \frac{\xi^2}{2}\right)\psi(\xi) \tag{5}$$

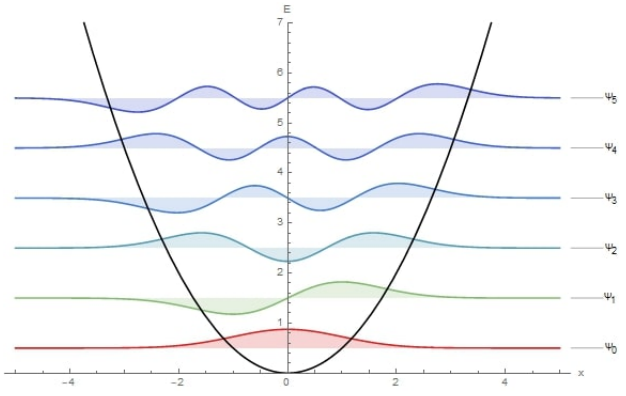

Figure 1: Wave functions

A formal analytical solution consists in extracting the asymptotic behaviour for large ξ with the minus sign (to avoid non physical quantities) and multiply it for $H(\xi)$, which is a well-behaved function for large ξ, usually a polynomial that is odd for odd n and even for even n. In this way the final wave function for the symmetric harmonic potential has n nodes and the same parity as n:

$$\psi_n(\xi) = H_n(\xi) \cdot e^{-\xi^2/2} \tag{6}$$

The corresponding allowed quantized energies are:

$$\varepsilon = n + \frac{1}{2} \tag{7}$$

It is now possible to find the specific functions $g(x)$ and $s(x)$ to perform the Numerov algorithm to solve equation (5), and their adimensional equivalent. In the `Fortran` implementation we inserted $s_n(x) = s_n(\xi) = 0$ and:

$$g_n(x) = \frac{2m}{\hbar^2}[E_n - V(x)] \ \longrightarrow\ g_n(\varepsilon) = \varepsilon - \frac{1}{2}\xi^2 \tag{8}$$

The auxiliary function f_n is introduced to simplify the writing:

$$f_n = 1 + g_n\frac{(\Delta\xi)^2}{12} \tag{9}$$

Also equation (3) is rewritten in a more compact and easy way, and inserted inside a loop in the code to calculate the wave function at each grid step $\xi_i = i \cdot \Delta\xi$.:

$$y_{n+1} = \frac{(12 - 10f_n)\ y_n - f_{n-1}\ y_{n-1}}{f_{n+1}} \tag{10}$$

This procedure implies the knowledge of E_n, necessary for the definition of g_n.

4 Code Implementation and Error Definition

4.1 Eigenvalue

The implemented program solves Schrödinger without knowing the analytical eigenvalue, but only the number of nodes of the researched wave function. For this reason a second loop is designed to find E values and evaluate them.
The procedure is similar to the Bisection Method: an iterative formula is performed until the current energy does match an eigenvalue, within an accuracy of `eps` $= 10^{-9}$. If the energy does not correspond to an eigenvalue, we would observe a divergence in $\psi(\xi)$, that corresponds to an non physical state, and would be eliminated.
This Shooting Method is used to choose the energy at each iteration starting from $E = (E_{max} - E_{min})/2$: the middle point of the upper or lower interval is chosen from time to time looking at the matching point of the two parts of the function, imposing the continuity of the first derivative. An outward and an inward Numerov integration are performed indeed respectively in the range $[0, x_c]$ and from x_{max} to x_c, which is the classical point of inversion.
The energy is lowered or raised depending on whether the number of crossing in the first half of the function (in the classically forbidden zone there won't be any) is too high or too low compared to `nodes`.
Then the Taylor expansions of y_L and y_R is calculated, subtracted and another change of variable is performed $y_i'' \equiv -g_i\ y_i + s_i$ to obtain:

$$y_i'^R - y_i'^L = \frac{y_{i-1}^L + y_{i+1}^L - (14 - 12\ f_i)\ y_i}{\Delta\xi} + O[\Delta\xi^2] \tag{11}$$

In this way, if this discontinuity is positive, the energy is too high, and we will have to choose the half-lower interval, otherwise the upper-half. After this evaluation the continuity of the wave function is imposed normalising to 1 and re-scaling by a factor $y_L(x_c)/y_R(x_c)$.

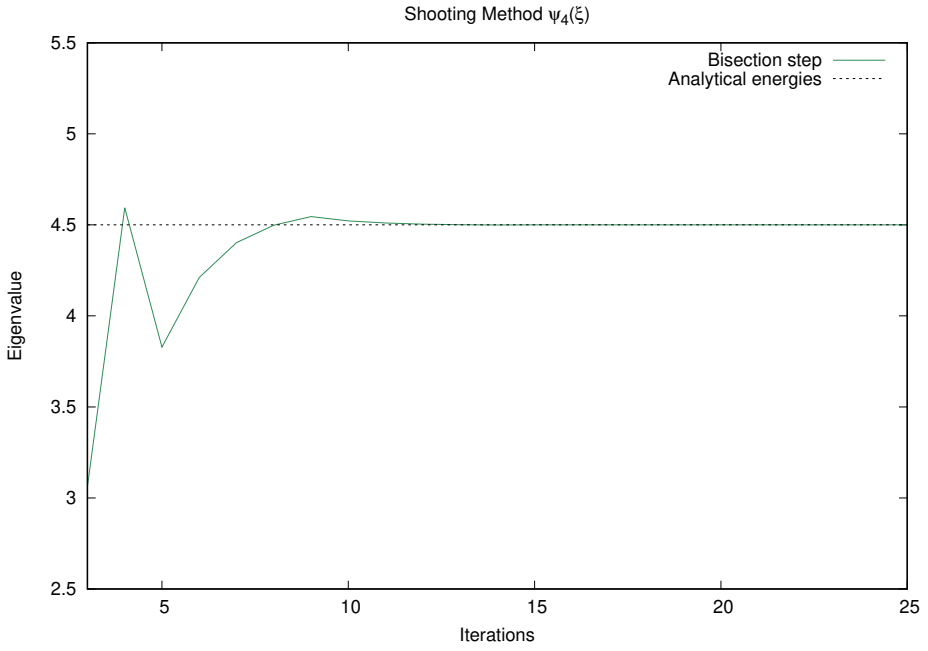

Figure 2: 4 nodes, $N = 500$

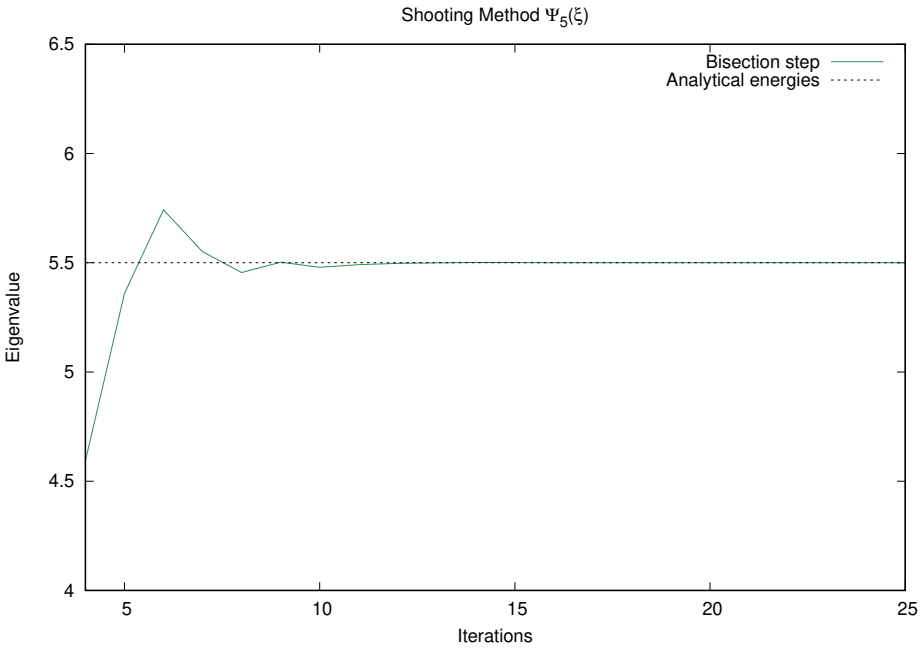

Figure 3: 5 nodes, $N = 500$

In the previous images the eigenvalue convergence to the correct E_n via the Shooting Method is reported; the chosen wave function parameters are `nodes` $= 4, 5$ and `x_{max}` $= 7$; the convergence at 4.5 and 5.5 is visible in both cases and happens in only 10 to 20 steps.

4.2 Eigenfunction

As regards the wave function, taking into account equation (6), the one for four and five nodes is searched. As said, the initial conditions are of fundamental importance in starting correctly the Numerov algorithm; the programs is initialized with:

For odd n:

1. $y(\xi_0) = 0.0$
2. $y_1(\xi_0) = \Delta\xi$

For even n:

1. $y(\xi_0) = 1.0$
2. $y_1(\xi_0) = \frac{(12-10\ f_0)\ y_0}{2f_1}$

In the following images, the squared wave functions are reported in function of the discretization step; the integration is performed only for positive values of ξ, because negative ones are obtained through symmetry. In each case the solution in superimposed to the correct analytical one from the literature, where the Hermite polynomials are respectively:

$$H_4(\xi) = 16\xi^4 - 48\xi^2 + 12 \tag{12}$$

$$H_5(\xi) = 32\xi^5 - 160\xi^3 + 120\xi \tag{13}$$

The results for classical probability are plotted in green together with the other ones. As expected, the quantum particle has non zero probability in certain classically forbidden regions; also has a local maximum in zero, while the classical ρ_{cl} has a local minimum there. Anyway, the Numerov Algorithm seems to work appropriately.

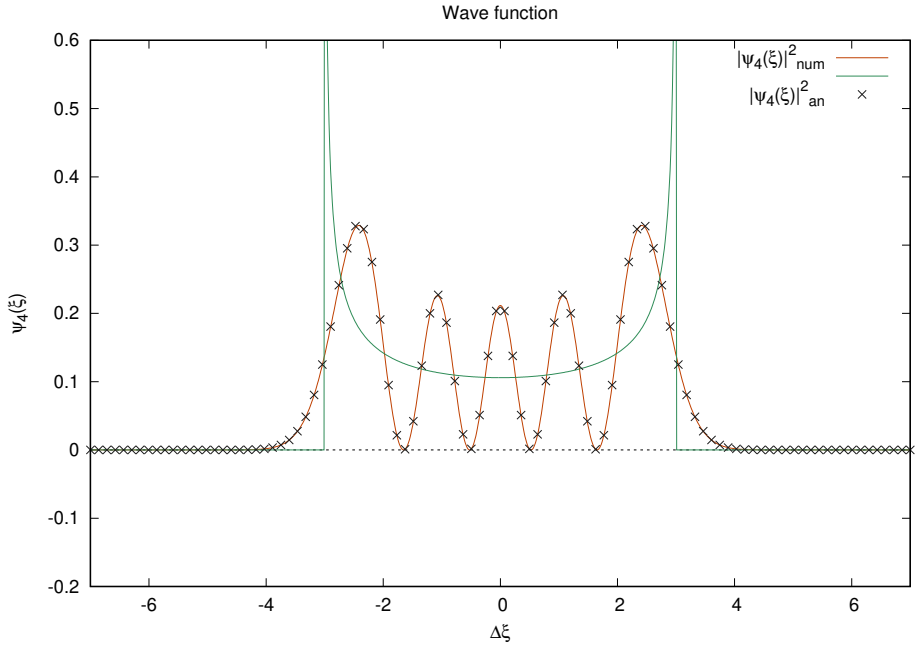

Figure 4: Four nodes and $N = 500$

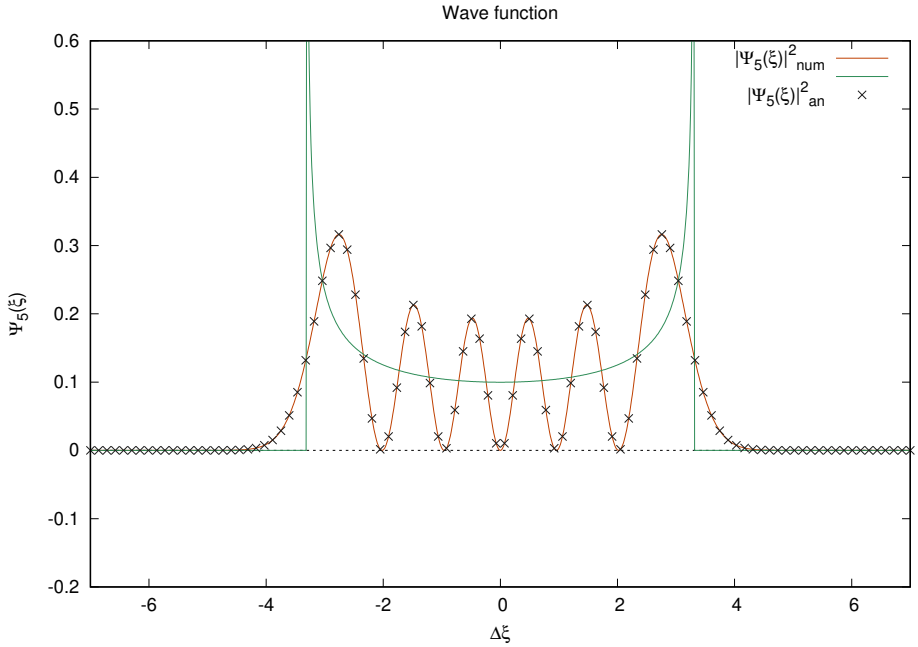

Figure 5: Five nodes and $N = 500$

5 Global Error Dependence from the Step

Another very important parameter is `mesh`, which is the number of considered grid points; in the code it spans from 100 to 2000 with a step of 20, and allowed us to study the Numerov's results and accuracy for different grid densities.
First of all the error was defined: the global error has been calculated as the difference in absolute value between the real analytical eigenvalue and the numerically calculated one. Given that to obtain the Numerov formula we expanded up to fifth order, the error is expected to go as $O(\Delta\xi^6)$.
It is important to consider that the integration runs over a grid whose points have a fixed range that after a big number of steps adds up like 2 ξ_{max}/h, so the actual global error should more precisely be expected to go as $O(\Delta\xi^5)$. Furthermore, other authors pointed out the possibility of the error to go as $O(\Delta\xi^4)$, as the Runge-Kutta Algorithm.
To evaluate this dependency, as said, an external loop is inserted to go over different grid densities, and the result of $|E_n - E|$ is plotted in function of the step for four and five nodes between $[-7, +7]$.

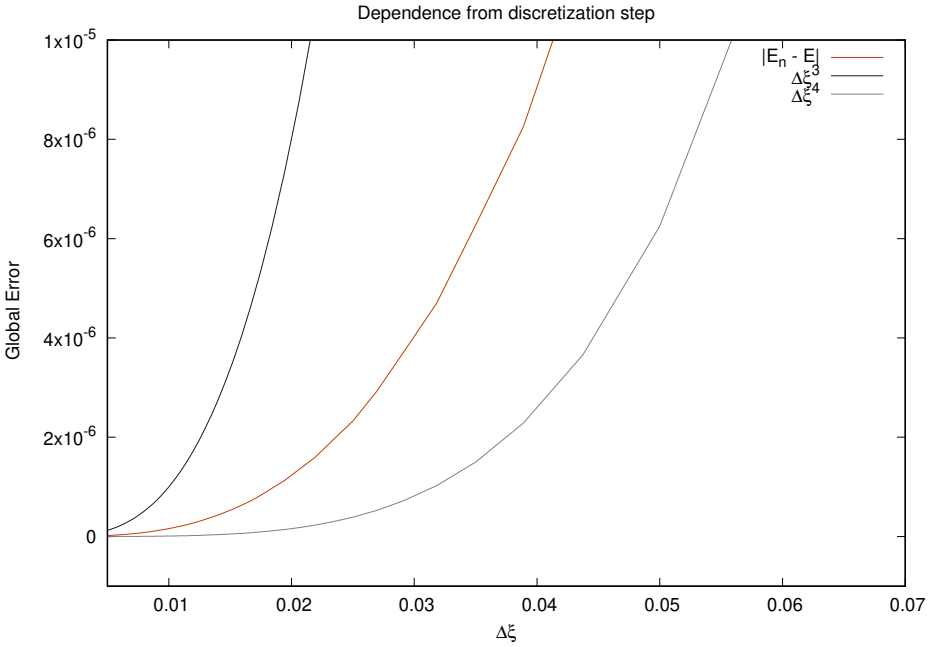

Figure 6: Global error for 4 nodes

From the achieved results, it is clear that the actual global error goes unexpectedly as $O(\Delta\xi^3)$: this means that somewhere in the code, a lower order of error is added to the theoretical prevision. We assumed that the round-off errors were not a problem given that we implemented the code for working in double precision. But this is actually not true.
This higher error is in fact to be imputed to a loss of precision in the computation of the second derivative; in the condition for the continuity in the code we used:

$$\psi(\xi_i \pm \xi_i) \equiv \psi_{i\pm1} \simeq \psi(\xi_i) \pm \Delta\xi\ \psi'(\xi_i) + \frac{1}{2}(\Delta\xi)^2\ \psi''(\xi_i) + O(\Delta\xi^3) \tag{14}$$

Summing these two equivalences the second derivative is determined by:

$$\psi''(\xi_i) = \frac{\psi(\xi_{i+1}) + \psi(\xi_{i-1}) - 2\ \psi(\xi_i)}{(\Delta\xi)^2} \tag{15}$$

In the limit where $\Delta\xi$ is very small, the approximation becomes better, but a truncation error is introduced: we are subtracting two quantities with finite precision (15 significant digits) that are increasingly similar one to the other; the smaller the discretization step, the bigger the limiting factor we are introducing. This is the mechanism responsible to the loss of precision compared to the expected one.

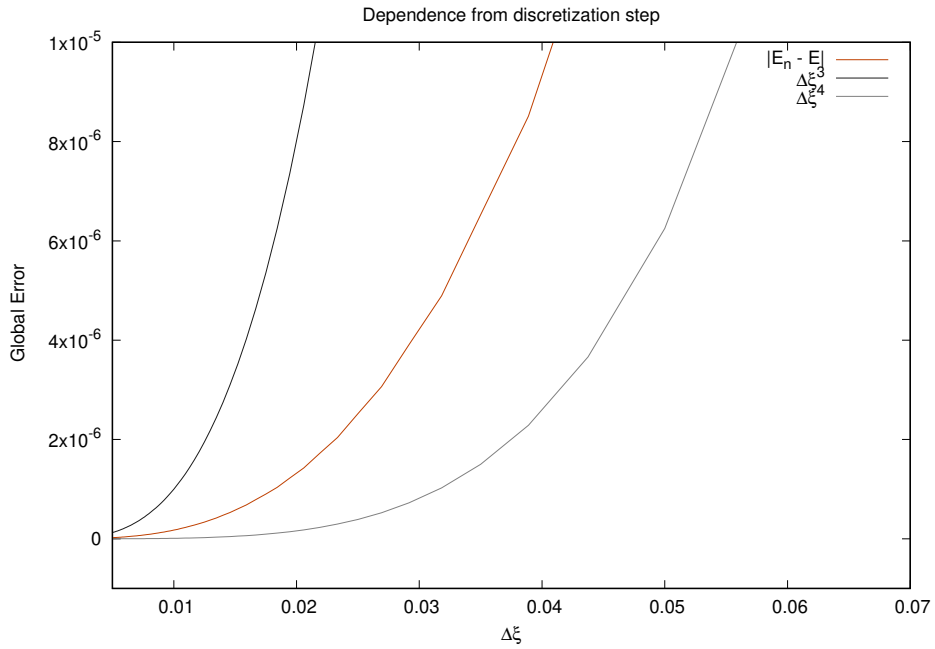

Figure 7: Global error for 5 nodes

6 Possible Improvement

To lower this effect of the discretization step, a different strategy to calculate the energy is experimented. The same code is used with the difference that E_i are now calculated with perturbative theory. The input parameters are the same, but only the wave function $\psi_4(\xi)$ has been considered. As in `hydrogen_radial.f90`, the adimensional difference between the current eigenvalue and the correct one is estimated in first order perturbation theory and considered the global error of the problem. In the code the grid is equispaced and not logarithmic as in the original draft. Also here we deal with the fact that the first derivative is discontinuous in the classical inversion point `icl`. So the Numerov algorithm gives a different result for taking `icl` as central point (y_{icl})) or `icl` ± 1 (y_{cusp}).
Then a variation of the function f is calculated, from which a those of the potential and the energy:

$$\delta e = \langle \psi | \delta V | \psi \rangle = -\frac{12}{(\Delta\xi)^2} \, |y(\xi_c)|^2 \, \Delta\xi \, \delta f \tag{16}$$

In this equation δf is considered the variation of the f function of the Numerov method from the value of the same function for a different problem where a delta function in superimposed (with a normalization constant) at $\xi_c \equiv \xi_{icl}$ generating a discontinuity:

$$V_{new} = v_0 \, \delta(\xi - \xi_{icl}) \tag{17}$$

As in the previous part of the exercise, the δe sign is considered for the Shooting Method, the same procedure is performed for different grid density values, and the global error (with the same definition as before) is plotted in function of the step:

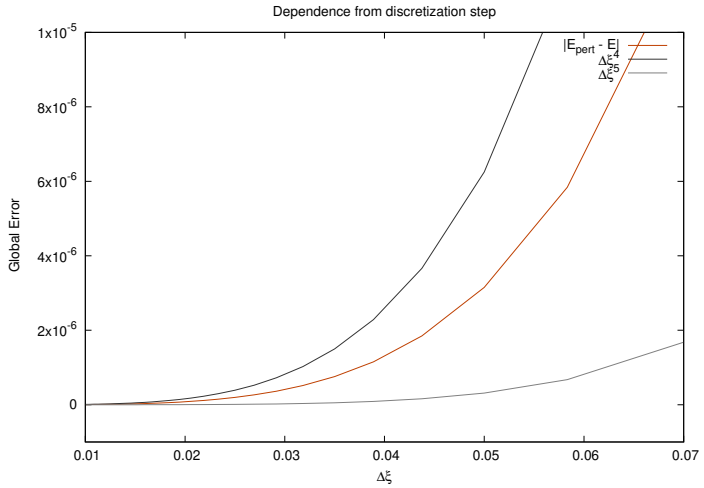

Figure 8: Four nodes, N = 500

This time the accuracy goes like $O(\Delta\xi)^4$, which is better then the previous result, this demonstrate that the new way of calculating the energy is more effective, because in the perturbative treatment we are not calculating second derivatives or subtracting similar quantities as in the previous case.

References

[1] Peter Young, "Numerov method for integrating the one-dimensional Schrödinger equation.", Physics 115/242

[2] Paolo Giannozzi, "Numerical Methods in Quantum Mechanics", University of Udine, A.A. 2021/2022