# NUMEROV METHOD ANALYSIS WITH A GOAL OF APPLICATION OF COMPLEX PLASMA MODELS

**Nenad M. Sakan**[1] **and Zoran Simić**[2]

[1]Institute of Physics Belgrade Pregrevica 118, Belgrade, Serbia
[2]Astronomical Observatory Volgina 7, P.O.Box 74 11060 Belgrade, Serbia nsakan@ipb.ac.rs

## 1 Radial part of the Schrödinger equation

$$-\frac{\hbar^2}{2m}\left(\frac{1}{r^2}\frac{d}{dr}\left(r^2\frac{dR}{dr}\right)-\frac{l(l+1)}{r^2}R(r)\right)+V(r)R(r)=ER(r). \quad (1)$$

After introducing a new functions $R(r) = P(r)/r$, $\tilde{V}(r) = V(r) + (\hbar^2/2m)(l(l+1)/r^2)$, simplifies the form of the radial part

$$-\frac{\hbar^2}{2m}\frac{d^2P(r)}{dr^2}+\tilde{V}(r)P(r)=EP(r). \quad (2)$$

### 1.1 Numerov method for radial Schrödinger equation

The Numerov method for 2 uses a Taylor expansion of the differential equation is used. If analyzig $q(r) = \tilde{V}(r) - E$, the equation $P''(r) = q(r)P(r)$ is solved. The Taylor expansion is valid for the linear mesh, e.g. $r_i = i * h$, where $P(r_i) \equiv P_i$ and $q(r_i) \equiv q_i$ :

$$P_{i+1}=\frac{12\left[2P_i-P_{i-1}\right]+h^2\left[10q_iP_i-q_{i-1}P_{i-1}\right]}{12-h^2q_{i+1}}-\frac{P_i^{(6)}h^6}{20\left(12-h^2q_{i+1}\right)}, \quad (3)$$

where $P_i^{(n)} \equiv \frac{d^n}{dr^n}P(r_i)$. The first order differential is given by

$$\begin{aligned}P_i' = {} & \frac{1}{12h}\left[P_{i-2}-8P_{i-1}+8P_{i+1}-P_{i+2}\right]- \\ & \frac{h}{60}\left[q_{i-2}P_{i-2}-2q_{i-1}P_{i-1}+2q_{i+1}P_{i+1}-q_{i+2}P_{i+2}\right]-\frac{11}{2520}P_i^{(7)}h^7.\end{aligned} \quad (4)$$

In order to avoid the problems related to the accumulation of the numerical error a new variable is introduced, $x = x(r)$, $dx = x'(r)dr$. For the logarithmic grid a function is given by

$$x(r)=\log\left(\frac{Zr}{a_0}\right), \qquad \Delta x=\frac{a_0}{Zr}\delta r. \quad (5)$$

in order for system to be solvable by a Numerov method on a different grid $x_i = x_0 + h * i$. In a case of logarithmic grid a function $y(x) = P(r(x))/\sqrt{r(x)}$ neutralizes the first order differential and preserves a form of differential equation $y''(x) = q(r(x))y(x)$, solvable by a Numerov method.

$$V_{Coul}(r)=-\frac{1}{r}, \qquad V_{Cut}(r)=\begin{cases}-\frac{1}{r}+\frac{1}{r_{Cut}} & : r<r_{cut}\\ 0 & : r\geq r_{cut}\end{cases} \quad (6)$$

## 2 Test procedure and results

The analysis is performed using the Coulomb potential, e.g. the solution are for the hydrogen atom without the influence of the plasma, since the stability is expected to be the same with more complex pseudo potentials and the Coulomb one have an analytical and known solutions. As it is known, the convergence of the potential and physical meaning of the wave function led to asymptotic solutions used for the initial values of the numerical solution presented by

$$R(r)|_{r\to 0}\sim r^l, \qquad P(r)|_{r\to 0}\sim r^{l+1}, \quad (7)$$

and for the large values of $r$

$$R(r)|_{r\to\infty}\sim r^{n-1}\exp\left\{-\frac{Zr}{na_0}\right\}, \qquad P(r)|_{r\to\infty}\sim r^{n}\exp\left\{-\frac{Zr}{na_0}\right\}. \quad (8)$$

With the help of varying parameter $\varepsilon$ the second bond value in both inward and outward integration is varied, mathematically could be presented as

$$\begin{aligned}&F_0=F_0, \qquad F_1^{NEW}=k*F_1, \qquad F_N=F_N, \qquad F_{N-1}^{NEW}=k*F_{N-1},\\ &F\equiv[R(r),P(r)] \qquad k=(1+\varepsilon), \qquad \varepsilon\in(-1,1)\end{aligned} \quad (9)$$

In this analysis a parameter $\varepsilon$ took values [$-0.1$, $-0.05$, $-0.01$, $-0.005$, $-0.001$, $0$, $0.001$, $0.005$, $0.01$, $0.05$, $0.1$]. All of these parameter values, in exception of $-0.1$, that are smaller or equal to $0$, led to the same energy values with the relative error smaller than $10^{-5}$. In the case of the smallest values for $\varepsilon > 0$ the result yields a lower energy state, otherwise the numerical solution will be colapsed. The accuracy of the numerical procedure could be seen on Figure 1.

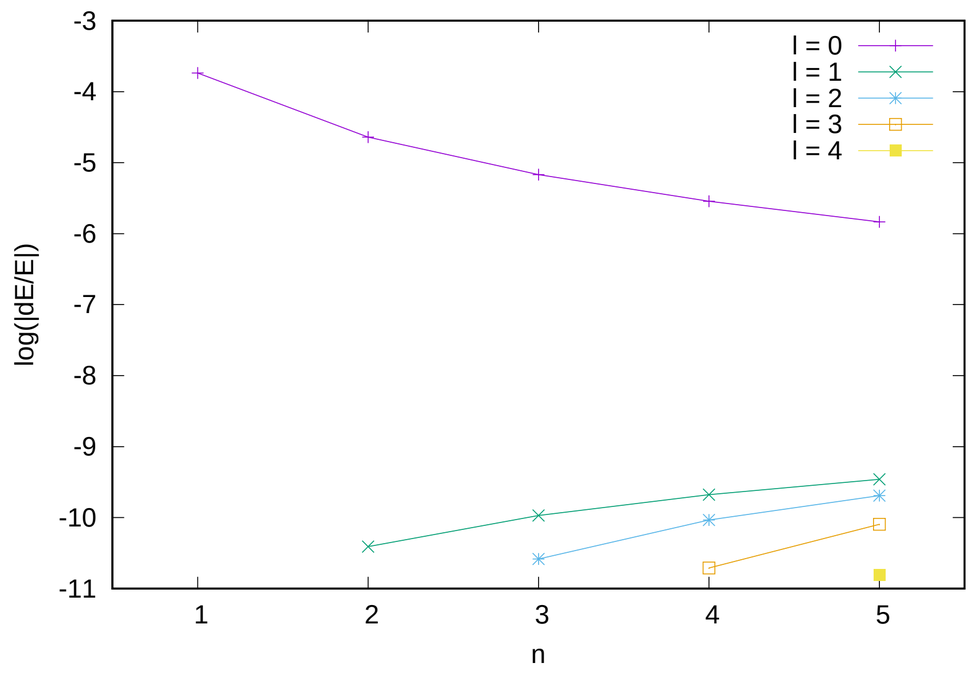


**Figure 1.** The absolute relative error of energy determination using Numerov method logarythmic grid numerical solution for radial part of Coulomb potential.

## 3 CONCLUSION

The numerical integration method, particularly the Numerov type integration method with logarithm and $1/r^3$ grid could be used for solving of model potential of dense hydrogen plasma, Havlová et al., 1984. The analysis of the stability of the solution with the initial values on the Coulomb potential led us to conclusion that the model is also usable for cut-off Coulomb model potential. The method possesses fast convergence toward to a solution, and is very applicable when using it in more complex analysis, as well as for coupling with molecular dynamics codes. Even more, it gave an opportunity to solve more complex model potential to describe different atoms in dense plasma. The further analysis is needed for avoiding of numerical errors in solution, as well as to optimize for a best mesh densities selection.


- Adamyan V. M., Djurić Z., Ermolaev A. M., Mihajlov A. A., Tkachenko I. M.: 1994, J.Phys.D, **27**, pp 111–118.
- Adamyan V. M., Djurić Z., Mihajlov A. A., Sakan N. M., Tkachenko I. M.: 2004, J.Phys.D., **37**, pp. 1896–1903.
- Fortov V. E., Iakubov I. T.: 1989, Physics of Nonideal Plasma, Hemisphere, New York
- Havlová, H., Smrčka, L.: 1984, Czech J Phys **34**, pp. 961–968. DOI: 10.1007/BF01589825
- Kobzev G., Jakubov I., Popovich M. (Eds.): 1995., Transport and Optical Properties of Non-Ideal Plasmas, Plenum Press, New York, London
- Mihajlov A. A., Sakan N. M., Srećković V. A., Vitel Y., 2011, Baltic Astron. **20**, p. 604
- Noumerov, B. V.: 1924, MNRAS **84**, 8., pp 592-602, DOI:10.1093/mnras/84.8.592
- Paolo Giannozzi, 2012/2013, Numerical Methods in Quantum Mechanics, Corso di Laurea Magistrale in Fisica Interateneo Trieste
- Sakan N. M.: 2010, Journal of Physics: Conference Series, **257**, nov, p 012036
- Sakan, N.M., Srećković, V.A., Simić, Z.J., Dimitrijević, M.S. : 2018, Atoms **6**, 4
- Srećković V. A., Ignjatović L. M., Mihajlov A. A., Dimitrijević M. S.: 2010, MNRAS, **406** 590–596.