Publ. Astron. Obs. Belgrade No. 99 (2020), 311 - 314 *Contributed Paper*

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*
E–mail nsakan@ipb.ac.rs

[2] *Astronomical Observatory Volgina 7, P.O.Box 74 11060 Belgrade, Serbia*

Abstract. The dense plasma is a complex system, with it's specifics in describing of related to more common plasma systems. It is proven that a Cut-off coulomb model potential had it's advantages in describing of the hydrogen plasma of moderate up to the higher plasma non ideality. The need for introducing a more complex models of atom in plasma is needed. The further modification and development of a similar or more advanced model potentials is expected to produce a better and more applicable results. There is a need for fast and accurate enough method of their solution. In this paper the analysis of the logarithmic grid of Numerov method for solving a Hydrogen Coulomb potential is analyzed.

1. THEORY

Moderate and high density plasma is characterized by the strong inter particle forces, leading to the coupling of the charged species in plasma, see Fortov et al. 1989, Kobzev et al. 1995., Adamyan et al. 1994 and Adamyan et al. 2004 for example. In order to characterize a non ideality the parameter Γ is defined by

$$\Gamma = \frac{\langle E_{Coul} \rangle}{kT_e} = \frac{q_e^2}{4\pi\varepsilon_0 kT_e} \sqrt[3]{\frac{4\pi n_e}{3}}, \tag{1}$$

for the plasma of temperature T_e and density n_e, note that in the local thermodynamical equilibrium an electron temperature and electron density could be used. Non ideality parameter itself presenting a ratio of Coulomb inter particle interaction in compare to average thermal energy of the plasma system. The Γ parameter for slightly and moderately non ideal plasma is within orders of 0.1 up to 10.

The plasma, as a collective phenomena, could be analyzed in a quantum mechanical approach, as a single particle which potentials is influenced by all the plasma species. The particle-plasma interaction is therefore described with the help of the pseudo potential. Having in mind that the closest neighbors reflect onto the mid range zone of the potential, where Coulomb potential weakness in comparison to their influence, while average plasma influence reflects as a constant potential level in a far field region. The cut-off Coulomb potential presents a good description of plasma influence in close vicinity of the analyzed particle, as well as in far field zone, so the

more complex forms of the pseudo potential is needed, see Mihajlov et al. 2011, Sakan 2010, Sakan et al. 2018 and Srećković et al. 2010. In general the potential of arbitrary form does not posses an analytical solution, so that numerical method for solution of a Schrödinger equation is needed.

In this paper an initial analysis of the stability of the numerical solution method took a place. As a main candidate the Numerov method with the logarithmic grid is selected.

1. 1. RADIAL PART OF THE SCHRÖDINGER EQUATION

In description of the plasma atom interaction a radial part of Schrödinger equation is used in order to calculate the radiative parameters of plasma

After introducing a new function $R(r) = P(r)/r$ into the radial part of the Schrödinger equation, as well as the use of a modified potential $\tilde{V}(r) = V(r) + (\hbar^2/2m)(l(l+1)/r^2)$, simplifies the form of the radial part

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

1. 2. NUMEROV METHOD FOR RADIAL SCHRÖDINGER EQUATION

The differential equation 2 is solvable with the help of Numerov method behind which a Taylor expansion of the differential equation is used. If the new function $q(r) = \tilde{V}(r) - E$, the differential equation tooks the form $P''(r) = q(r)P(r)$. Having in mind that the Taylor expansion is valid for the linear mesh, e.g. $r_i = i * h$, where the notation $P(r_i) \equiv P_i$ and $q(r_i) \equiv q_i$ is used here. As it is known a solution for the radial function P_i is given by

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

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

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

More details about the application of the Numerov procedure from Noumerov 1924, and the application onto the radial Schrödinger equation could be seen in Paolo Giannozzi 2012/2013 and Havlová et al. 1984. It could be seen from the previous equations that an error of the Numerov method could be estimated easily and is well behaved in most of the radial part of the function space. In order to avoid the problems related to the accumulation of the numerical error as well as to adopt for a more realistic grid for the differential equation that has to be solved, a new variable is introduced, $x = x(r)$, $dx = x'(r)dr$. For the logarithmic grid a function is given by

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

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.

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.

Here we applied the Numerov procedure method that uses two separate solution, outward integration, from the smallest radius values to the end of the classical solution zone, and other, inward integration, from the largest values of the radius down to the joining point. The solution is possible only for some values of the energy levels, so the shooting method is applied in order to search for the values of the bond state energy.

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

$$R(r)|_{r\to 0} \sim r^l, \qquad P(r)|_{r\to 0} \sim r^{l+1}, \tag{6}$$

and for the large values of r

$$R(r)|_{r\to \infty} \sim r^{n-1} \exp\left\{-\frac{Zr}{na_0}\right\}, \qquad P(r)|_{r\to \infty} \sim r^n \exp\left\{-\frac{Zr}{na_0}\right\}. \tag{7}$$

In order to study a stability of the procedure of variation of a second initial value is involved. With the help of varying parameter ε the second bond value in both inward and outward integration is varied, mathematically could be presented as

$$\begin{array}{cccc} F_0 = F_0, & F_1^{NEW} = k * F_1, & F_N = F_N, & F_{N-1}^{NEW} = k * F_{N-1}, \\ F \equiv [R(r), P(r)] & k = (1+\varepsilon), & \varepsilon \in (-1, 1) & \end{array} \tag{8}$$

In this analysis a parameter ε 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.

3. CONCLUSION

The preliminary test led a conclusion that 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. In analyzed cases there is an exact mathematical form of the wave function. 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 because of that 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

n	l	E_{calc}/E_H	dE/E
1	0	0.9998168	-0.0001832
2	0	0.9999084	-0.0000916
	1	1.0000000	0.0000000
3	0	0.9999387	-0.0000613
	1	1.0000000	0.0000000
	2	1.0000000	0.0000000
4	0	0.9999442	-0.0000458
	1	1.0000000	0.0000000
	2	1.0000000	0.0000000
	3	1.0000000	0.0000000
5	0	0.9999632	-0.0000368
	1	1.0000000	0.0000000
	2	1.0000000	0.0000000
	3	1.0000000	0.0000000
	4	1.0000000	0.0000000

Table 1: Calculated energy for the unmodified initial values.

model potential in order to describe different atoms in dense plasma. The further analysis is needed for development of a method for determination and avoid of numerical errors in solution, as well as to optimize a procedure for best mesh densities selection.

References

Adamyan, V. M., Djurić, Z., Ermolaev, A. M., Mihajlov, A. A., Tkachenko, I. M.: 1994, *J.Phys.D*, **27**, 111.

Adamyan V. M., Djurić Z., Mihajlov, A. A., Sakan, N. M., Tkachenko, I. M.: 2004, *J.Phys.D.*, **37**, 1896.

Fortov V. E., Iakubov I. T.: 1989, *Physics of Nonideal Plasma*, Hemisphere, New York

Havlová, H., Smrčka, L.: 1984, *Czech J Phys* **34**, 961.

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**, 604.

Noumerov, B. V.: 1924, *MNRAS* **84**, 8., 592.

Paolo Giannozzi: 2012/2013, lecture notes: *Numerical Methods in Quantum Mechanics*, Corso di Laurea Magistrale in Fisica Interateneo Trieste.

Sakan, N. M.: 2010, *Journal of Physics: Conference Series*, **257**, 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.