Studies of quantum self-frictional atomic potentials and nuclear attraction forces

I. I. Guseinov, B.A. Mamedov

Department of Physics, Faculty of Arts and Sciences, Onsekiz Mart University, Çanakkale, Turkey

Department of Physics, Faculty of Arts and Sciences, GaziosmanpaşaUniversity, Tokat, Turkey

E-mail: bamamedov@yahoo.com

Abstract

This paper is devoted to examine a physical nature of quantum self-frictional atomic potentials and nuclear attraction forces. Using analytical formulas for the $L^{(p_l^*)}$– generalized Laguerre polynomials ($L^{(p_l^*)}$-GLPs) and $\psi^{(p_l^*)}$- generalized exponential type orbitals ($\psi^{(p_l^*)}$-GETOs), the self-frictional atomic potentials and nuclear attraction forces are investigated, where $p_l^* = 2l + 2 - \alpha^*$ and α^* is the integer ($\alpha^* = \alpha, -\infty < \alpha \le 2$) or noninteger ($\alpha^* \ne \alpha, -\infty < \alpha^* < 3$) self-frictional quantum number. We notice that the $L^{(p_l^*)}$-GLPs, the origin of which is the quantum self-frictional fields, are the radial parts of the $\psi^{(p_l^*)}$-GETOs. The dependence of the quantum self-frictional potentials and nuclear attraction forces as a function of the distance from nucleus is analyzed. The relationships presented are valid for the arbitrary values of quantum numbers and scaling parameters.

Keywords: Self-frictional potentials, Self-frictional nuclear attraction forces, Laguerre polynomials, Exponential type orbitals

I. Introduction

The physical nature of particles is one of the most fundamental bases in not only understanding electronic structures of atoms and molecules, but also developing efficient and accurate structure methods of arbitrary matter. The role of quantum damping or self-frictional forces in natural sciences is to predict what can be observed and to provide an understanding of the observations. To extend the predictions of these forces to the domain of science, it is, therefore, necessary to use quantum mechanics for describing properties of arbitrary system.

According to the self-frictional theory introduced by Lorentz in classical electrodynamics [1-3], the electrons move around the atomic nuclei under total nuclear attraction forces $\vec{F}_L = \vec{F} + \frac{2e^2}{3c^3}\dddot{\vec{r}}$, where $\dddot{\vec{r}}$ is the time derivative of the acceleration of the electron. The analytical formulas for the quantum self-frictional nuclear attraction forces in

terms of $L^{(p_l^*)}$-GLPs and $\psi^{(p_l^*)}$-GETOs, suggested in (see Refs. [4, 5] and references therein), are the extensions of Lorentz theory to the quantum cases. In the quantum cases, atomic electrons move under nuclear attraction forceswhich depend on quantum numbers n,l,α^* and scaling parameters of orbitals. The origin of these forces is the quantum self-frictional fields which are analogous to the damping fields introduced by Lorentz. It should be noted that the quantum self-frictional theory is one of the greatest advances in modern physics.

We note that, in the case of disappearing quantum frictional fields, $\psi^{(p_l^*)}$ -GETOs and eigenvalues are reduced to the results obtained for the hydrogen-like atoms by Schrödinger in nonstandard convention. Therefore, the $\psi^{(p_l^*)}$-GETOs become noncomplete, i.e., $\psi_{nlm}^{(p_l^*)} = \psi_{nlm}$. Here, the ψ_{nlm} is Schrödinger's wave function in nonstandard convention.

The purpose of this work is, using formulas for $L^{(p_l^*)}$-GLPs and $\psi^{(p_l^*)}$-GETOs, to construct the self-frictional atomic potentials and nuclear attraction forces for $1 \le n < \infty$, $0 \le l \le n-1$, $-\infty < \alpha^* < 3$ and arbitrary values of screening constants of orbitals. The $\psi^{(p_l^*)}$ -GETOs can be used for wide applications in structure calculations of atomic, molecular, nuclear and solid systems.

2. Theory

The atomic potentials and forces based on the use of $L^{(p_l^*)}$-GLPs have the following forms [4]:

self-frictional atomic potentials

$$V_{nl}^{(p_l^*)}(\zeta, r) = -\frac{\zeta n}{r} U_{nl}^{(p_l^*)}(t) \tag{1}$$

$$U_{nl}^{(p_l^*)}(t) = U_{q_n^*-(p_l^*+1)}^{(p_l^*+1)}(t) = 1 + \frac{\alpha^* - 1}{n} \frac{L_{q_n^*-(p_l^*+1)}^{(p_l^*+1)}(t)}{L_{q_n^*-p_l^*}^{(p_l^*)}(t)} \ , \tag{2}$$

self-frictional nuclear attraction forces

$$F_{nl}^{(p_l^*)}(\zeta, r) = -\frac{\zeta n}{r^2} G_{nl}^{(p_l^*)}(t) \tag{3}$$

$$G_{nl}^{(p_l^*)}(t)=1+\frac{\alpha^*-1}{n}\frac{L_{q_n^*-(p_l^*+1)}^{(p_l^*+1)}(t)}{L_{q_n^*-p_l^*}^{(p_l^*)}(t)}\left[1-t\left(\frac{L_{q_n^*-(p_l^*+1)}^{(p_l^*+1)}(t)}{L_{q_n^*-p_l^*}^{(p_l^*)}(t)}-\frac{L_{q_n^*-(p_l^*+2)}^{(p_l^*+2)}(t)}{L_{q_n^*-(p_l^*+1)}^{(p_l^*+1)}(t)}\right)\right] \tag{4}$$

Here, $t=2\zeta r,\ p_l^*=2l+2-\alpha^*,\ \ q_n^*=n+l+1-\alpha^*$ and $q_n^*-p_l^*=n-(l+1)$. The $L^{(p_l^*)}$-GLPs in Eqs.(2) and (4) are defined as

$$L_{nl}^{(p_l^*)}(t)=L_{q_n^*-p_l^*}^{(p_l^*)}(t)=\frac{\Gamma(q_n^*+1)}{(q_n^*-p_l^*)!\Gamma(p_l^*+1)}\,{}_1F_1(-[q_n^*-p_l^*];p_l^*+1;t), \tag{5}$$

where ${}_1F_1$ is the confluent hypergeometric function [6],

$${}_1F_1(-[q_n^*-p_l^*];p_l^*+1;t)=\sum_{k=0}^{q_n^*-p_l^*}\frac{(-[q_n^*-p_l^*])_k}{(p_l^*+1)_k}\frac{t^k}{k!}. \tag{6}$$

The quantities $(-[q_n^*-p_l^*])_k$ and $(p_l^*+1)_k$ in Eq.(6) are Pochhammer symbols.

It is easy to show that the number of infinite and minimal values of self-fictional potentials and nuclear attraction forces, respectively, is determined by

$$Y_{nl}^{(p_l^*)}=n-(l+1)\qquad for\ \ \alpha^*\le 0\ \ and\ \ \alpha^*>0. \tag{7}$$

The characteristics of self-frictional atomic potentials and nuclear attraction forces for $1\le n\le 4,\ 0\le l\le n-1,\ \ \alpha^*=-0.5\ \ and\ \ \alpha^*=1.5$ are demonstrated in Figures 1-9.

3. Results and Discussion

As can be seen from the equations presented in this study, the quantum self-frictional atomic potentials and nuclear attraction forces can be calculated with the help of formulas based on the use of $L^{(p_l^*)}$-GLPs. To do this, we need only the values of quantum numbers n,l,α^* and scaling parameter ζ. Using these relations, we constructed programs that are performed in the Mathematica 7.0 software package.

The properties of the self-frictional potentials and nuclear attraction forcesas a function of distance from nucleus for $1\le n\le 4,\ 0\le l\le n-1,\ \ \alpha^*=-0.5\ \ and\ \ \alpha^*=1.5$ are shown in Figures (1-9). These figures show that the number of infinite and minimal values of potentials and forces, respectively, is obtained by theuse of relation $Y_{nl}^{(p_l^*)}=n-(l+1)$ and therefore, the

atomic particle makes oscillation around these crucial points. It is seen from Figs. (1-9) that, in the case of $l = 0$,the self-frictional potentials and nuclear attraction forces takein the crucial points the maximum number of infinite and minimal values, respectively, and the values of these quantities decrease with increases in l and for $l = n-1$ disappear. In Fig. 1, the potentials and nuclear attraction forces defined in nonstandard convention are also shown. The dependence of crucial points from quantum numbers and scaling parameters is shown in Tables 1 and 2.

It should be noted that the presented formulas can be also used for evaluating self-frictional potentials and nuclear attraction forces with arbitrary values of quantum numbers ($1 \le n < \infty,\ 0 \le l \le n-1,\ -\infty < \alpha^* < 3$) and orbital parameter ($0 < \zeta < \infty$). We show, for the first time, that the quantum mechanical approach of evaluating self-frictional theory by extending Lorentz's damping theory which is also efficient and promising for the studies of understanding electronic structures of atoms and molecules.

References

1. H. A. Lorentz, The Theory of Electrons, Dover, New York (1953).
2. W. Heitler, The Quantum Theory of Radiation, Oxford University Press, Oxford University (1950).
3. L. D. Landau, E. M. Lifshitz, The Classical Theory of Fields, Pergamon, New York (1987).
4. I. I. Guseinov, in Sixth International Conference of the Balkan Physical Union in AIP Conference Proceedings, ed. by S.A. Cetin, *American Institute of Physics Conference Proceeding*, 899 (2007) 65.
5. B.A. Mamedov, Israfil I. Guseinov: A Pioneer of the quantum theory of atomic, molecular and nuclear systems, Int. J. Quantum Chem., 114 (2014) 361.
6. W. Magnus, F. Oberhettinger, R.P. Soni, Formulas and Theorems for the Special Functions of Mathematical Physics, New York, Springer (1966).

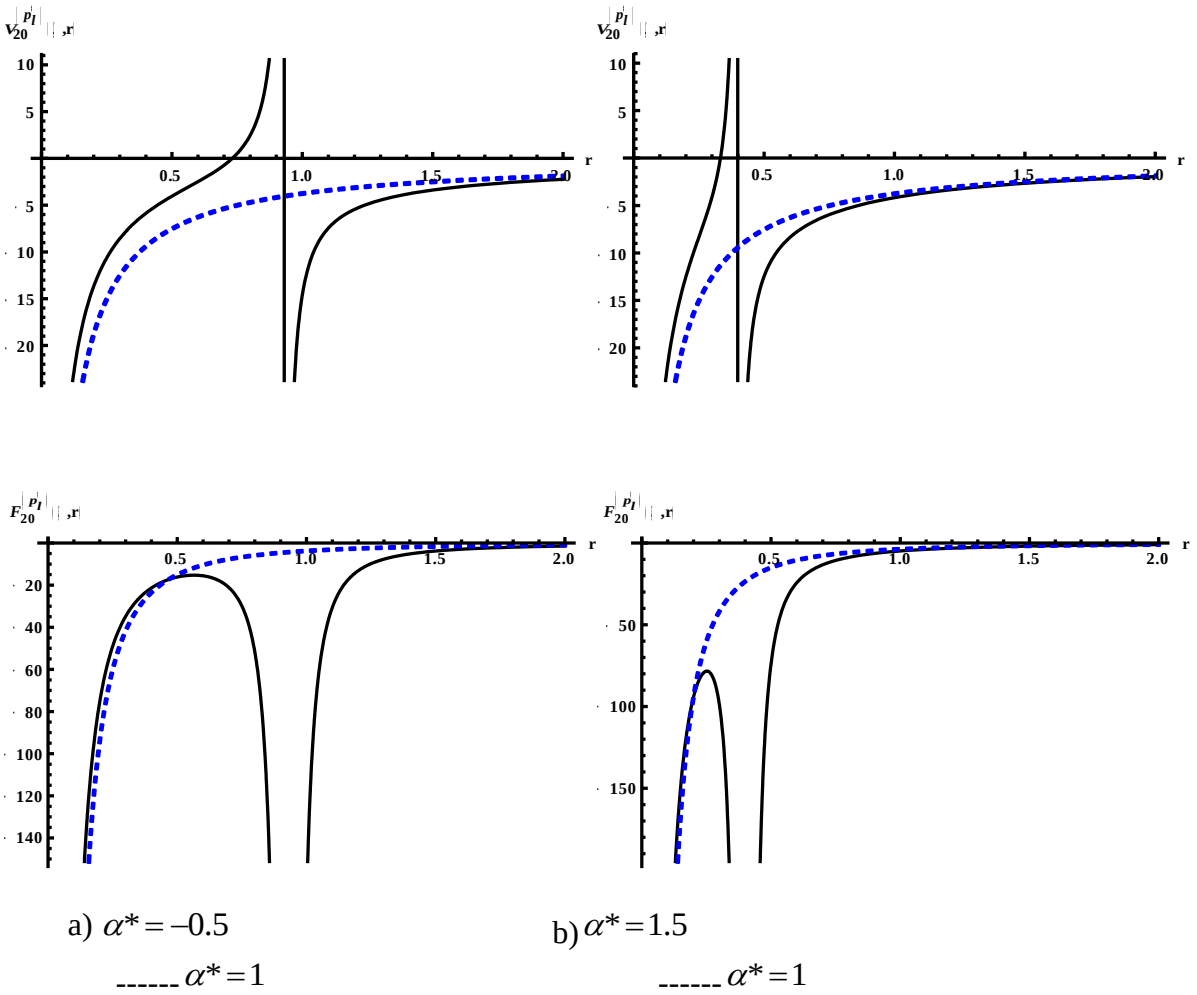


Fig. 1. Theself-frictional potentials and nuclear attraction forces as a function of distance from nucleus for $n=2, l=0$ and $\zeta=1.88$ $\left(Y_{10}^{(p_l^*)}=1\right)$

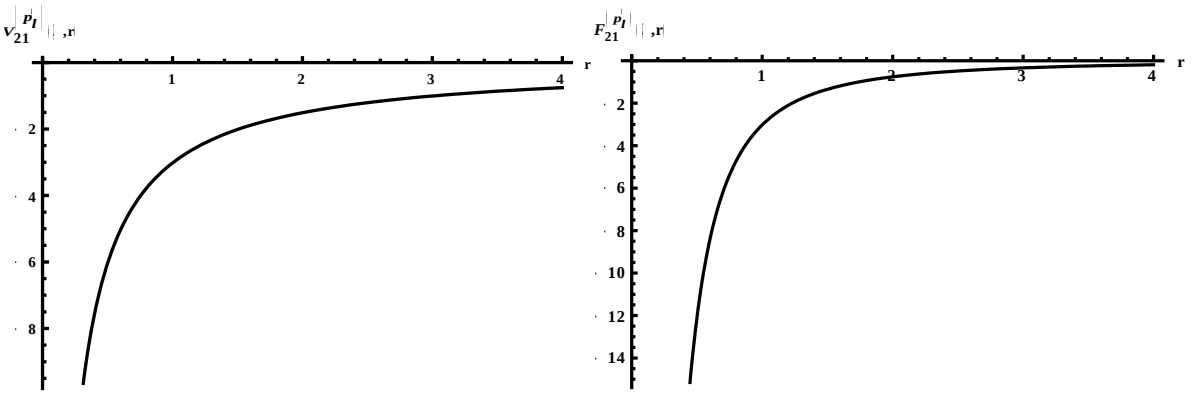
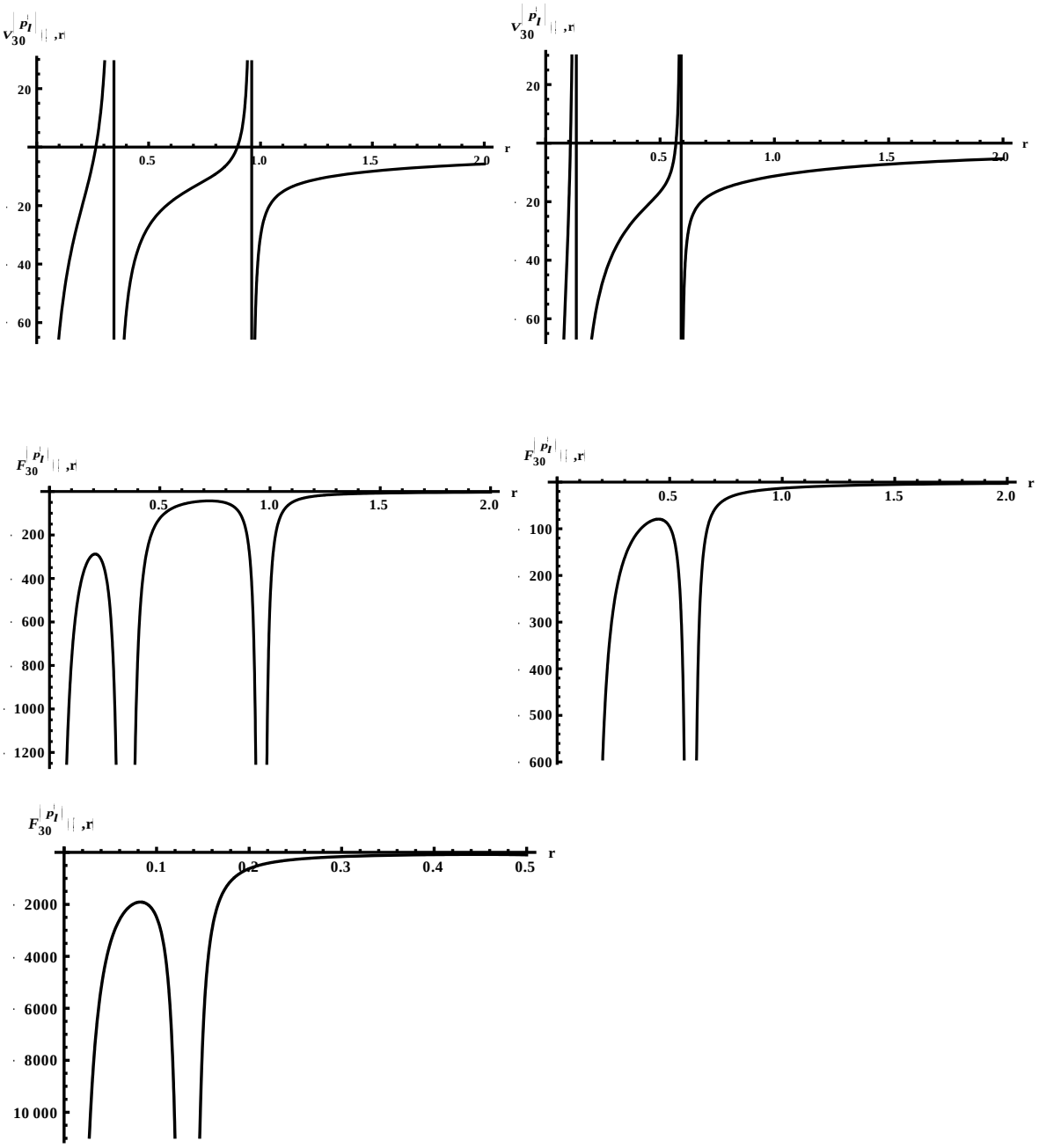
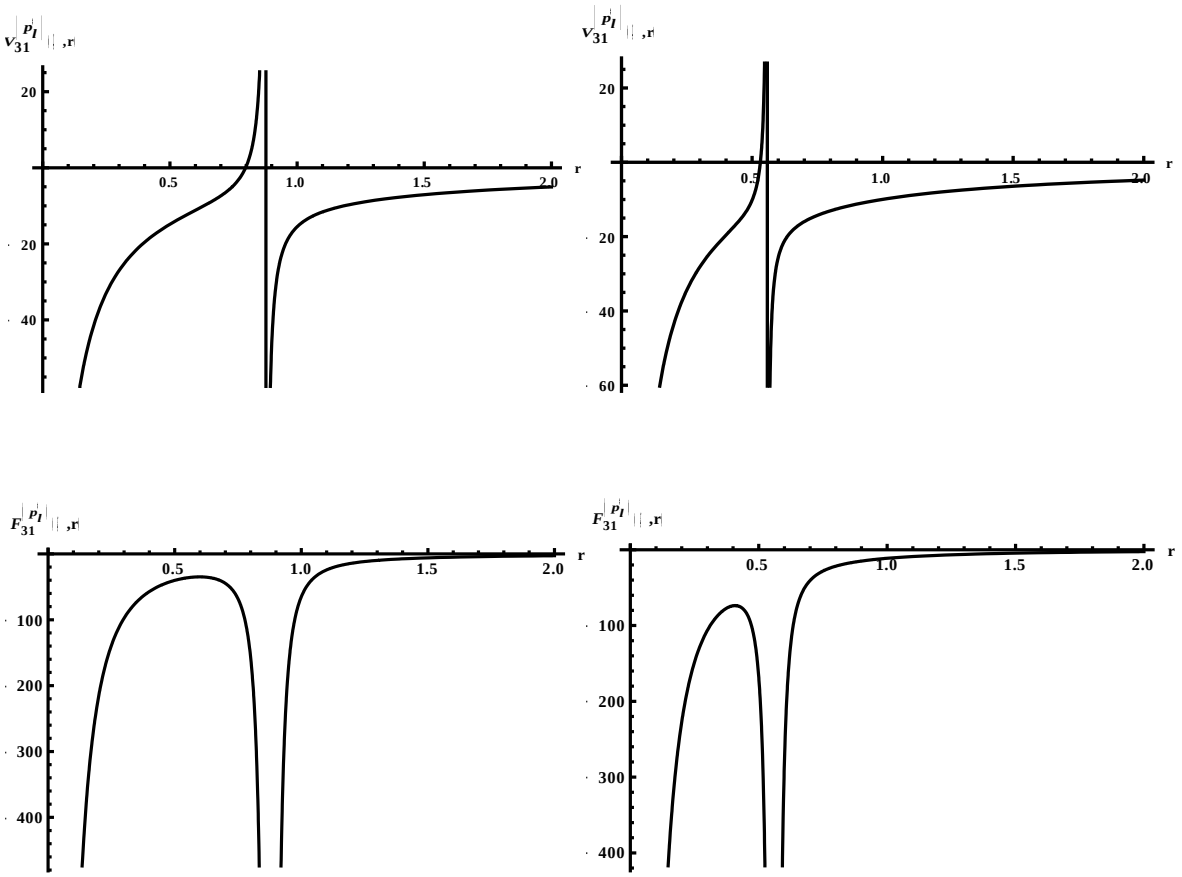


Fig. 2. The self-frictional potentials and nuclear attraction forces as a function of distance from nucleus for $n=2, l=1, \alpha^*=-0.5, \alpha^*=1.5$ and $\zeta=1.51$ $\left(Y_{21}^{(p_l^*)}=0\right)$



a) $\alpha^* = -0.5$ b) $\alpha^* = 1.5$

Fig. 3. The self-frictional potentials and nuclear attraction forces as a function of distance from nucleus for $n = 3, l = 0$ and $\zeta = 3.4466$ $\left(Y_{30}^{(p_l^*)} = 2\right)$



a) $\alpha^* = -0.5$ b) $\alpha^* = 1.5$

Fig. 4. The self-frictional potentials and nuclear attraction forces as a function of distance from nucleus for $n = 3, l = 1$ and $\zeta = 3.1354$ $\left(Y_{31}^{(p_l^*)} = 1\right)$

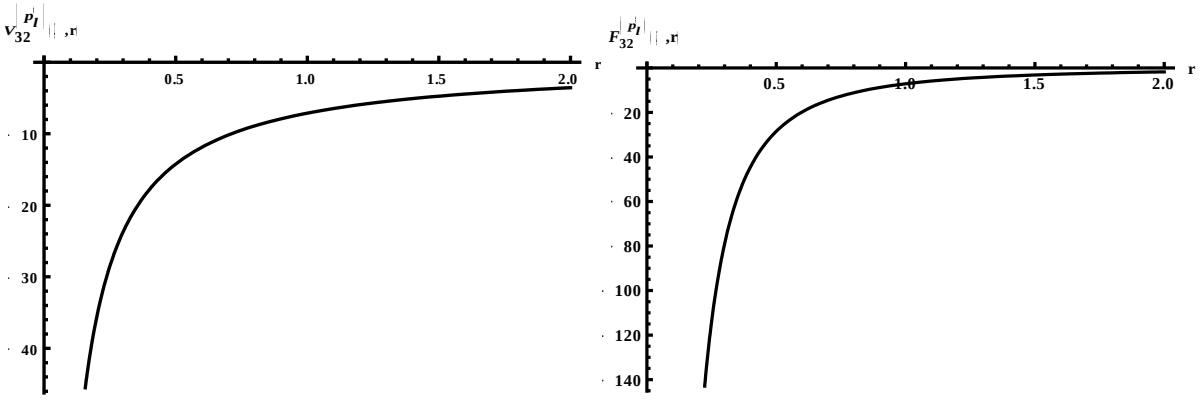
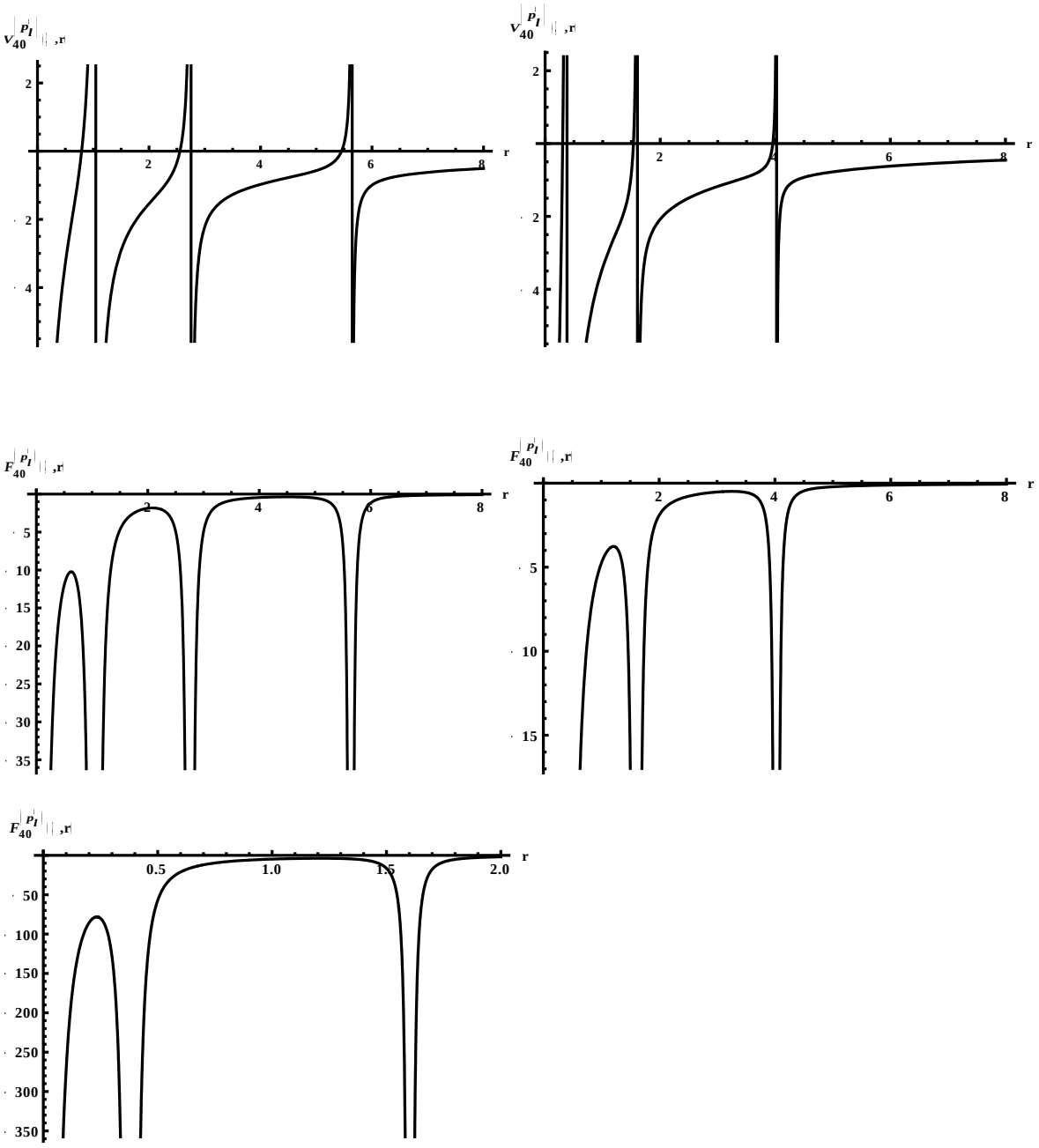
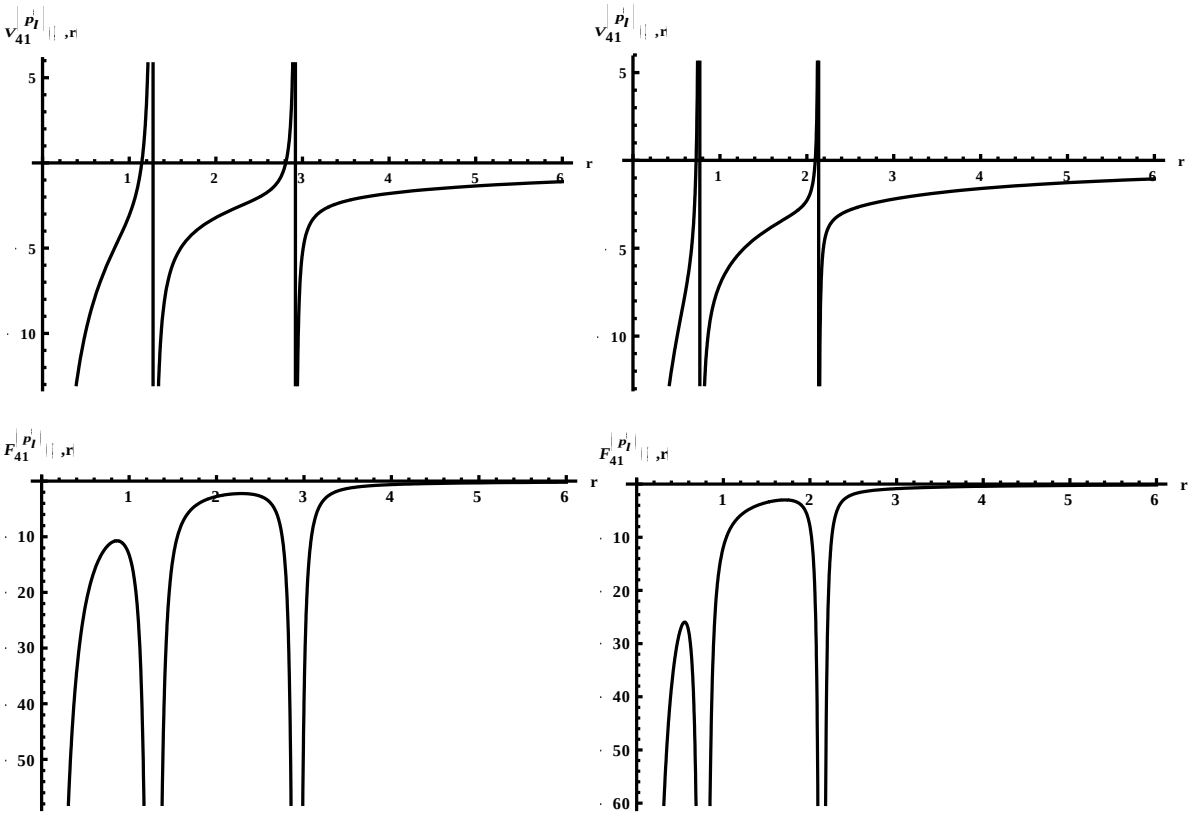


Fig. 5. The self-frictional potentials and nuclear attraction forces as a function of distance from nucleus for $n = 3, l = 2, \alpha^* = -0.5, \alpha^* = 1.5$ and $\zeta = 2.3733$ $\left(Y_{32}^{(p_l^*)} = 0\right)$



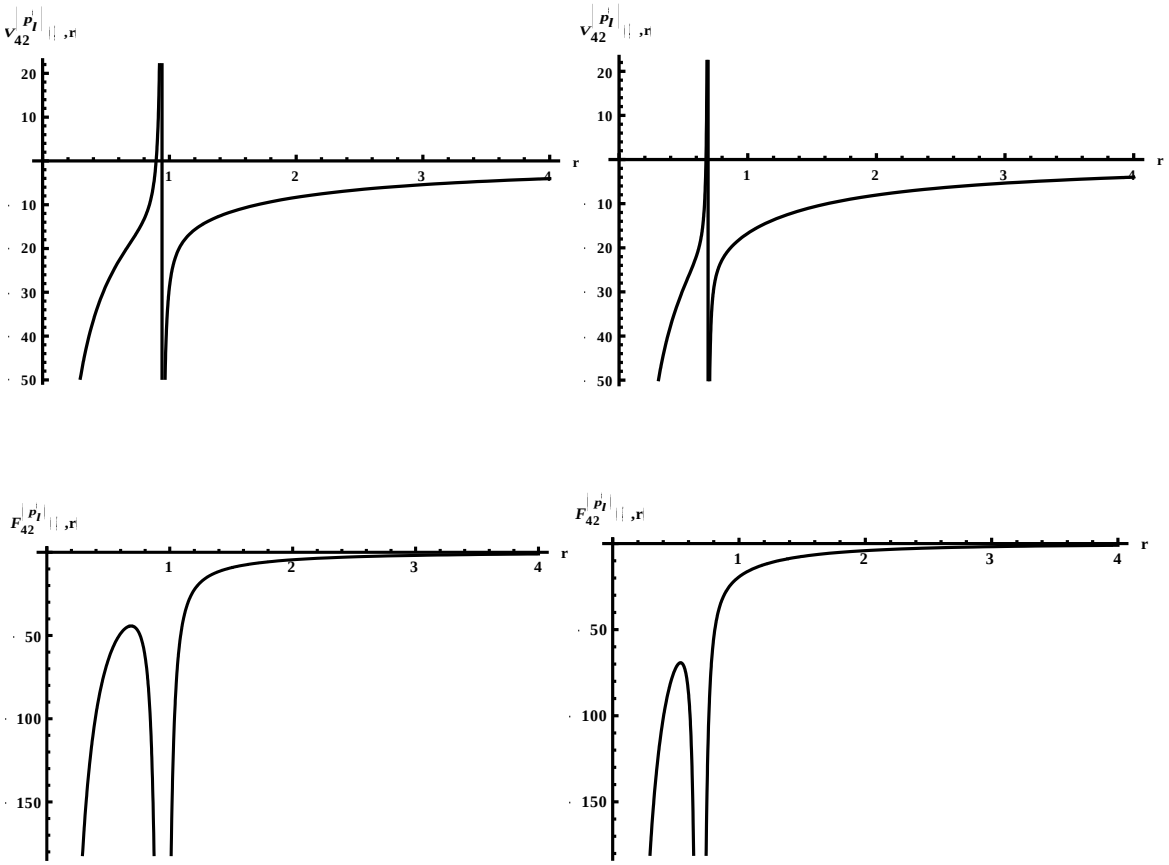
a) $\alpha^* = -0.5$ b) $\alpha^* = 1.5$

Fig. 6. The self-frictional potentials and nuclear attraction forces as a function of distance from nucleus for $n = 4, l = 0$ and $\zeta = 0.8733$ $\left(Y_{40}^{(p_l^*)} = 3\right)$



a) $\alpha^* = -0.5$ b) $\alpha^* = 1.5$

Fig. 7. The self-frictional potentials and nuclear attraction forces as a function of distance from nucleus for $n = 4, l = 1$ and $\zeta = 1.55$ $\left(Y_{41}^{(p_l^*)} = 2\right)$



a) $\alpha^* = -0.5$ b) $\alpha^* = 1.5$

Fig. 8. The self-frictional potentials and nuclear attraction forces as a function of distance from nucleus for $n = 4, l = 2$ and $\zeta = 3.98$ $\left(\left(Y_{42}^{(p_l^*)} = 1\right)\right.$

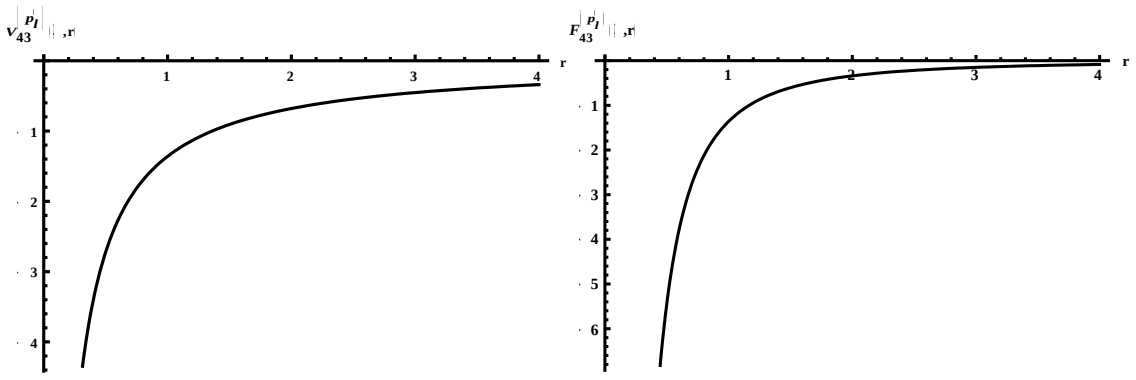


Fig. 9. The self-frictional potentials and nuclear attraction forces as a function of distance from nucleus for $n = 4, l = 3, \alpha^* = -0.5, \alpha^* = 1.5$ and $\zeta = 0.34$ $\left(\left(Y_{43}^{(p_l^*)} = 0\right)\right.$

Table1. Thevalues of crucial points for $1 \le n \le 4,\ 0 \le l \le n-1$ and $\alpha^* = -0.5$

n	l	ζ	r_1	r_2	r_3
2	0 1	1.88 1.51	0.5647		
3	0 1 2	3.4466 3.1354 2.3733	0.2072 0.5991	0.7244	
4	0 1 2 3	0.8738 1.55 3.98 0.34	0.6241 0.8612 0.6854	2.0831 2.2868	4.5156

Table 2. The values of crucial points for $1 \le n \le 4,\ 0 \le l \le n-1$ and $\alpha^* = 1.5$

n	l	ζ	r_1	r_2	r_3
2	0 1	1.88 1.51	0.2518		
3	0 1 2	3.4466 3.1354 2.3733	0.0825 0.4079	0.4217	
4	0 1 2 3	0.8738 1.55 3.98 0.34	0.2339 0.5543 0.5375	1.2119 1.7118	3.2575