Indian J Phys (March 2021) 95(3):405–410
https://doi.org/10.1007/s12648-019-01657-7

ORIGINAL PAPER

Application of quantum self-frictional nonperturbative theory for the study of atomic anharmonic oscillator potentials and their arbitrary derivatives

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Received: 02 February 2019 / Accepted: 30 September 2019 / Published online: 23 December 2019

Abstract: The self-frictional (SF) nonperturbative theory, introduced by one of the authors, is used for the evaluation of the $V^{(p_l^*)}$ and $V^{(\alpha^*)}$ atomic anharmonic oscillator potentials and their derivatives, where $p_l^* = 2l + 2 - \alpha^*$ and α^* represent the integer ($\alpha^* = \alpha,\ -\infty < \alpha \leq 2$) or non-integer ($\alpha^* \neq \alpha,\ -\infty < \alpha^* < 3$) SF quantum numbers. This study is based on the use of complete sets of $L^{(p_l^*)}$ and $L^{(\alpha^*)}$ SF polynomials. The dependence of the potentials and their derivatives from the nucleus distances is investigated. All of the obtained results are valid for the arbitrary values of quantum numbers, scaling parameters and SF quantum numbers.

Keywords: Self-frictional polynomials; Anharmonic oscillators; Nonperturbative theory

PACS Nos.: 03.65.-w; 31.10.+z; 31.15.xp

1. Introduction

The significant problem of accurately calculating atomic anharmonic oscillator potentials arises in the application of the nonperturbative theory introduced by Dyson [1–3], who provided an argument as to why perturbation series in quantum electrodynamics (QED) are divergent. The Dyson nonperturbative theory has seen a series of successful applications in QED [4–14] and string theory [15] and explores two- and four-dimensional gauge dynamics [16]. Accordingly, in the study of the anharmonic oscillator, a necessity arises for developing a self-frictional (SF) nonperturbative theory.

Based on these viewpoints, the investigation of classical and quantum SF fields is important for studying the behavior of electrons in atoms, since they are important for the accurate study of the atomic and molecular structures of substances. A significant and independent exploration of the theory of classical SF force was carried out by Lorentz, who produced explicit expressions for atomic nuclear forces based on the assumption that SF properties correspond to an appropriate interaction potential function, as obtained in Refs. [17–19]. Lorentz showed for the first time that for the nonrelativistic case, considering the own field effect of the electron (SF or damping), leads to the following total nuclear attraction force equation for the electron's motion around the nuclei:

$$\vec{F} = \vec{F}_N + \vec{F}_L; \quad \vec{F}_L = \frac{2e^2}{3c^3}\dddot{\vec{r}}, \tag{1}$$

where $\dddot{\vec{r}}$ is the time derivative of the acceleration of the electron [17]. One of the authors of this study firstly proposed the quantum theory of an SF field by developing Lorentz's classic damping theory, where the electrons move around the nuclei under two kinds of fields: nuclear attraction and SF fields [20–22]. It was found that the obtained formula for the quantum SF potential is in terms of $L^{(\alpha^*)}$ and $L^{(p_l^*)}$ generalized Laguerre polynomials and SF quantum numbers. Note that, in the case of a disappearing SF field, the SF potential reduces to the nuclear Coulomb potential.

It is well known that one of the methods of determining other physical properties according to the formulae representing the potential field is the consideration of a Taylor expansion of the potential around its equilibrium point

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[23]. Each term in the series expression allows the determination of other physical quantities corresponding to the potential field. The aim of this work is to use the quantum SF nonrelativistic nonperturbative theory for the investigation of the series expansion relations of the $V^{(p_l^*)}$ and $V^{(\alpha^*)}$ atomic anharmonic oscillator potentials (AAOPs) and their derivatives.

2. Definition and basic formulae

The following relations are used to study the AAOPs and their derivatives [24]:

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

$$U_{nl}^{(p_l^*)}(t) = 1 + \left(\frac{\alpha^*-1}{n}\right) q_n^* \frac{\mathcal{L}_{n-1\,l}^{(p_l^*+1)}(t)}{\mathcal{L}_{nl}^{(p_l^*)}(t)} \tag{3}$$

$$V_{nl}^{(\alpha^*)}(\zeta,r) = -\frac{\zeta n}{r} U_{nl}^{(\alpha^*)}(t) \tag{4}$$

$$U_{nl}^{(\alpha^*)}(t) = 1 + \left(\frac{\alpha^*-1}{n}\right) \sqrt{2n(n-(l+1))}\, \frac{\mathcal{L}_{n\,l+1}^{(\alpha^*+1)}(t)}{t\mathcal{L}_{nl}^{(\alpha^*)}(t)}, \tag{5}$$

where

$$\mathrm{L}_{nl}^{(p_l^*)}(t) = \frac{\Gamma(q_n^*+1)}{(n-(l+1))!\Gamma(p_l^*+1)}\, {}_1F_1\left(-[n-(l+1)];p_l^*+1;t\right) \tag{6}$$

$$= \frac{\Gamma(q_n^*+1)}{(n-(l+1))!} \sum_{\eta=l+1}^{n} \tilde{a}_{n\eta}^{(p_l^*)l} t^{\eta-(l+1)} \tag{7}$$

$$\mathrm{L}_{nl}^{(\alpha^*)}(t) = \left[\frac{\Gamma(q_n^*+1)}{(2n)^{\alpha^*}(n-(l+1))!}\right]^{\frac{1}{2}} \frac{t^l}{\Gamma(p_l^*+1)}\, {}_1F_1(-[n-(l+1)];p_l^*+1;t) \tag{8}$$

$$= \left[\frac{\Gamma(q_l^*+1)}{(2n)^{\alpha^*}(n-(l+1))!}\right]^{\frac{1}{2}} \sum_{\eta=l+1}^{n} \tilde{a}_{n\eta}^{(\alpha^*)l} t^{\eta-1} \tag{9}$$

$$\tilde{a}_{n\eta}^{(p_l^*)l} = \tilde{a}_{n\eta}^{(\alpha^*)l} = \frac{(-[n-(l+1)])_{\eta-(l+1)}}{\Gamma(p_l^*+1)(p_l^*+1)_{\eta-(l+1)}[\eta-(l+1)]!} \tag{10}$$

and $t = 2\zeta r$, ζ is the screening constant $(0<\zeta<\infty)$, $p_l^* = 2l+2-\alpha^*, q_n^* = n+l+1-\alpha^*$ and ${}_1F_1$ is the confluent hypergeometric function [25].

The definition of phases in this study [26] for the complex spherical harmonics $(Y_{lm_l}* = Y_{l-m_l})$ differs from the Condon–Shortley phases [27] by the sign factor $(-1)^{m_l}$.

3. Study of AAOPs and their derivatives

The SF AAOPs and their arbitrary derivatives are determined by the following relations:

$$V_{nl}^{(\delta^*)}(\zeta,r) = \frac{r^2}{2!}V_{nl}^{0(\delta^*)}(\zeta,r) + \frac{r^3}{3!}V_{nl}^{1(\delta^*)}(\zeta,r) + \frac{r^4}{4!}V_{nl}^{2(\delta^*)}(\zeta,r) + \cdots = \sum_{v=0}^{\infty} V_{nl}^{v(\delta^*)}(\zeta,r)\frac{r^{v+2}}{(v+2)!} \quad \text{for} \quad (\delta^*) = (p_l^*) \quad \text{or} \quad (\delta^* = \alpha^*), \tag{11}$$

where $p_l^* = 2l+2-\alpha^*$. Here, the functions $V_{nl}^{v(\delta^*)}(\zeta,r)$ for $v=0$ are determined by Eqs. (2)–(5). Using Eqs. (2)–(5), it is easy to show that the derivatives of potentials for $v=1$ and $v=2$ are defined as follows:

$$V_{nl}^{1(p_l^*)}(\zeta,r) = -\frac{\zeta n}{r^2}\left(1 + \left(\frac{\alpha^*-1}{n}\right) q_n^* \frac{\mathrm{L}_{n-1l}^{(p_l^*+1)}(t)}{\mathrm{L}_{nl}^{(p_l^*)}(t)} \left\{1 + t\left[q_n^* \frac{\mathrm{L}_{n-1l}^{(p_l^*+1)}(t)}{\mathrm{L}_{nl}^{(p_l^*)}(t)} - (q_n^*-1)\frac{\mathrm{L}_{n-2l}^{(p_l^*+2)}(t)}{\mathrm{L}_{n-1l}^{(p_l^*+1)}(t)}\right]\right\}\right) \tag{12}$$

$$V_{nl}^{2(p_l^*)}(\zeta,r) = -\frac{\zeta n}{r^3}\left\{2 + \left(\frac{\alpha^*-1}{n}\right) q_n^* \frac{\mathrm{L}_{n-1l}^{(p_l^*+1)}(t)}{\mathrm{L}_{nl}^{(p_l^*)}(t)} \left(2 + 2t\left((q_n^*-1)\frac{\mathrm{L}_{n-2l}^{(p_l^*+2)}(t)}{\mathrm{L}_{n-1l}^{(p_l^*+1)}(t)} - q_n^* \frac{\mathrm{L}_{n-1l}^{(p_l^*+1)}(t)}{\mathrm{L}_{nl}^{(p_l^*)}(t)}\right)\right.\right. + t^2\left((q_n^*-1)(q_n^*-2)\frac{\mathrm{L}_{n-3l}^{(p_l^*+3)}(t)}{\mathrm{L}_{n-1l}^{(p_l^*+1)}(t)} - 3q_n^*(q_n^*-1)\frac{\mathrm{L}_{n-2l}^{(p_l^*+2)}(t)}{\mathrm{L}_{nl}^{(p_l^*+1)}(t)} + 2(q_n^*)^2\left(\frac{\mathrm{L}_{n-1l}^{(p_l^*+1)}(t)}{\mathrm{L}_{nl}^{(p_l^*)}(t)}\right)^2\right)\left.\right\} \tag{13}$$

and

$$V_{nl}^{1\,(\alpha^*)}(\zeta,r) = -\frac{\zeta n}{r^2} \times \left(1-\left(\frac{\alpha^*-1}{n}\right)(n-(l+1))\left\{1-\frac{\mathrm{L}_{nl+1}^{(\alpha^*+1)}(t)}{t\mathrm{L}_{nl}^{(\alpha^*)}(t)}\left[\sqrt{\frac{2n}{n-(l+1)}}(p_l^*+2-t)-(2n)\frac{\mathrm{L}_{nl+1}^{(\alpha^*+1)}(t)}{\mathrm{L}_{nl}^{(\alpha^*)}(t)}\right]\right\}\right) \tag{14}$$

$$V_{nl}^{2\,(\alpha^*)}(\zeta,r) = -\frac{\zeta n}{r^3}\left\{2-\frac{1}{n}\left(\frac{\alpha^*-1}{n}\right)[2n(n-(l+1))]+\left(\frac{\alpha^*-1}{n}\right)\sqrt{2n(n-(l+1))}\frac{\mathrm{L}_{nl+1}^{(\alpha^*+1)}(t)}{t\mathrm{L}_{nl}^{(\alpha^*)}(t)} \times \left((2p_l^*-t+4)-\sqrt{2n(n-(l+1))}(p_l^*-t+3)\frac{\mathrm{L}_{nl+1}^{(\alpha^*+1)}(t)}{\mathrm{L}_{nl}^{(\alpha^*)}(t)}+\sqrt{2n(n-(l+1))}(p_l^*-t+2)\frac{\mathrm{L}_{nl+2}^{(\alpha^*+2)}(t)}{\mathrm{L}_{nl+1}^{(\alpha^*+1)}(t)}\right.\right.$$
$$\left.\left.-2\sqrt{[2n(n-(l+1))][2n(n-(l+2))]}\frac{\mathrm{L}_{nl+2}^{(\alpha^*+2)}(t)}{\mathrm{L}_{nl}^{(\alpha^*)}(t)}+2[2n(n-(l+1))]\left(\frac{\mathrm{L}_{nl+1}^{(\alpha^*+1)}(t)}{\mathrm{L}_{nl}^{(\alpha^*)}(t)}\right)^2\right)\right\} \tag{15}$$

Similar formulae for the derivatives of AAOPs can be also established for $3 \le v < \infty$.

In the case of the non-self-frictional (NSF) approximation (for $\alpha^* = 1,\ \zeta = \frac{Z}{n}$), the functions $V_{nl}^{v\,(p_l)}(\zeta,r)$ and $V_{nl}^{v\,(\alpha)}(\zeta,r)$ are defined as follows:

$$V_{nl}^{v\,(p_l^*)}(\zeta,r) = V_{nl}^{v\,(\alpha^*)}(\zeta,r) = -\frac{Z}{r^{v+1}}. \tag{16}$$

where $p_l = 2l+2,\ q_n = n+l+1$. The characteristics of the SF and NSF AAOPs and their derivatives for $1 \le Z \le 8$ are demonstrated in Figs. (1)–(8).

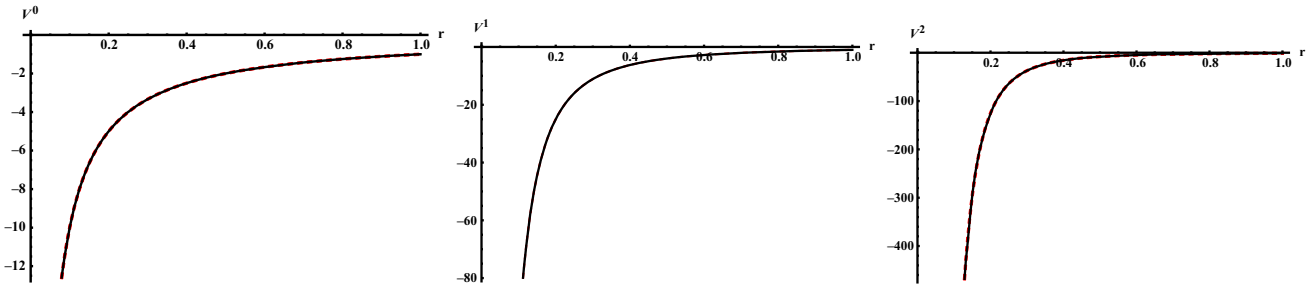

Fig. 1 Values of atomic anharmonic oscillator potential and its derivatives for $Z = 1$ with SF ($\alpha^* = 0.7,\ \zeta = 1.5,\ n = 1,\ l = 0$ and black color) and NSF ($\alpha^* = 1,\ \zeta = 1,\ n = 1,\ l = 0$ and red color) (color figure online)

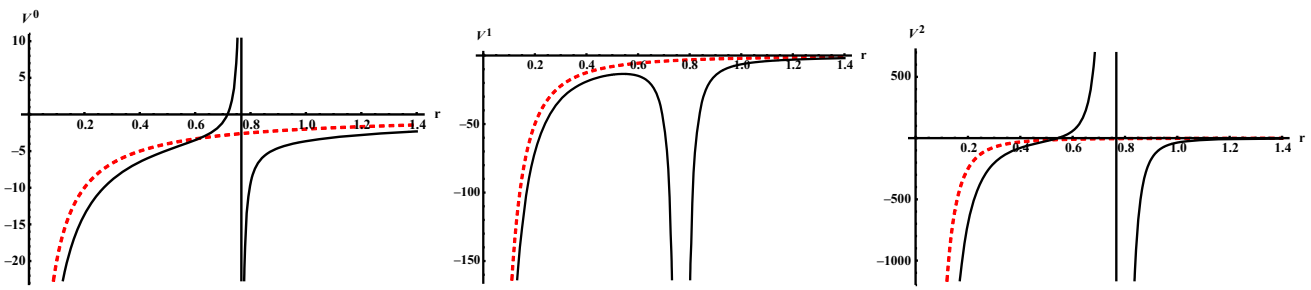

Fig. 2 Values of atomic anharmonic oscillator potential and its derivatives for $Z = 2$ with SF ($\alpha^* = 0.7,\ \zeta = 1.5,\ n = 2,\ l = 0$ and black color) and NSF ($\alpha^* = 1,\ \zeta = 1,\ n = 2,\ l = 0$ and red color) (color figure online)

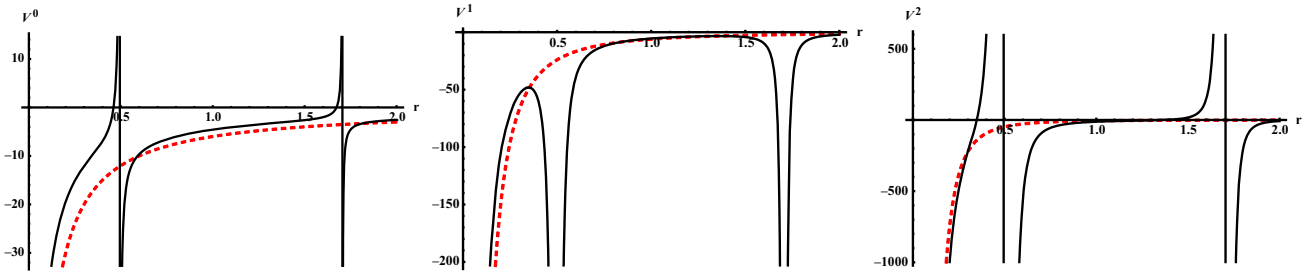

Fig. 3 Values of atomic anharmonic oscillator potential and its derivatives for $Z = 3$ with SF ($\alpha^* = 0.7,\ \zeta = 1.5,\ n = 3,\ l = 0$ and black color) and NSF ($\alpha^* = 1,\ \zeta = 2,\ n = 3,\ l = 0$ and red color) (color figure online)

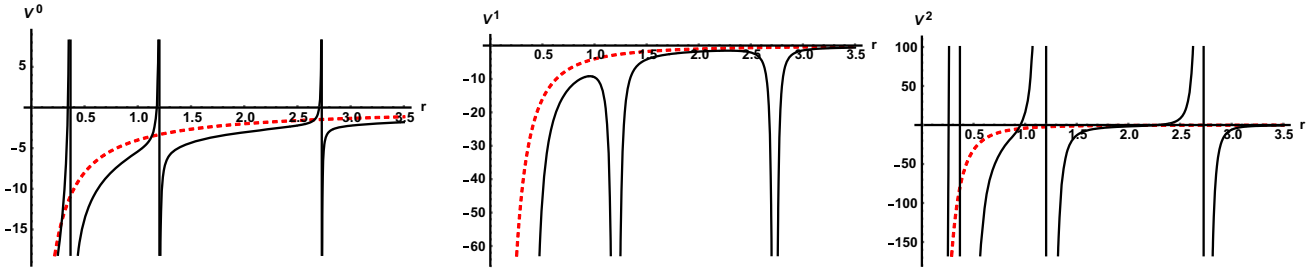

Fig. 4 Values of atomic anharmonic oscillator potential and its derivatives for $Z = 4$ with SF ($\alpha^* = 0.7,\ \zeta = 1.5,\ n = 4,\ l = 0$ and black color) and NSF ($\alpha^* = 1,\ \zeta = 1,\ n = 4,\ l = 0$ and red color) (color figure online)

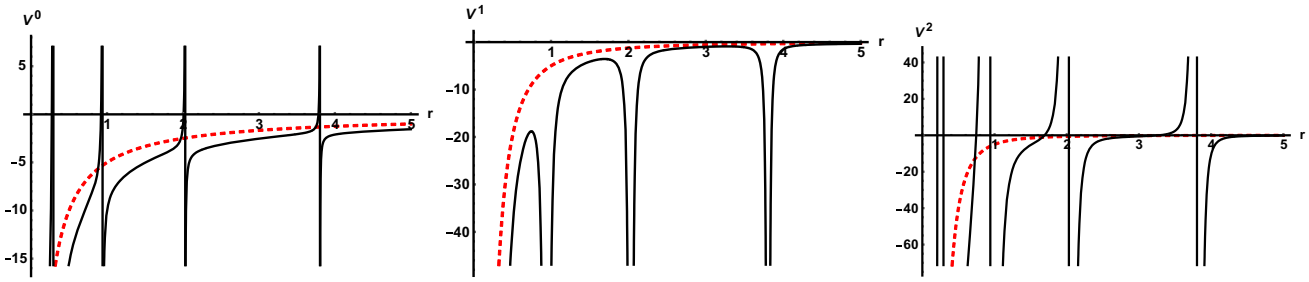

Fig. 5 Values of atomic anharmonic oscillator potential and its derivatives for $Z = 5$ with SF ($\alpha^* = 0.7,\ \zeta = 1.5,\ n = 5,\ l = 0$ and black color) and NSF ($\alpha^* = 1,\ \zeta = 1,\ n = 5,\ l = 0$ and red color) (color figure online)

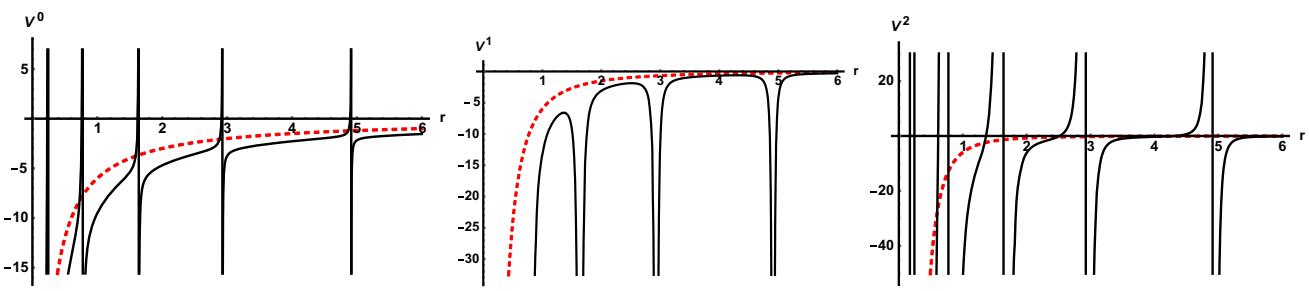

Fig. 6 Values of atomic anharmonic oscillator potential and its derivatives for $Z = 6$ with SF ($\alpha^* = 0.7,\ \zeta = 1.5,\ n = 6,\ l = 0$ and black color) and NSF ($\alpha^* = 1,\ \zeta = 1,\ n = 6,\ l = 0$ and red color) (color figure online)

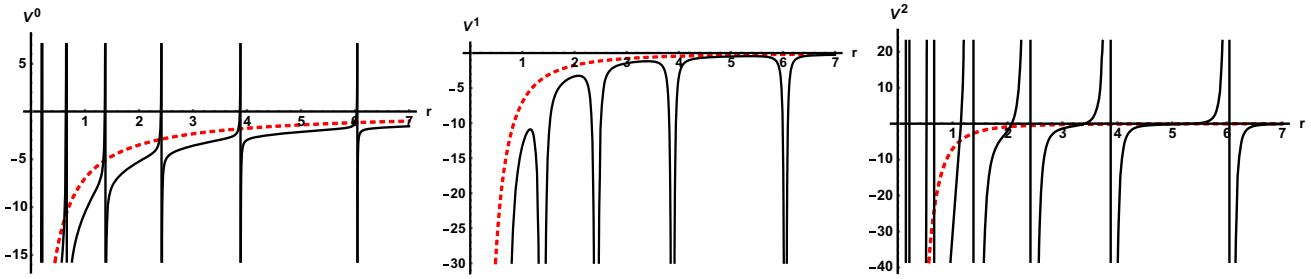

Fig. 7 Values of atomic anharmonic oscillator potential and its derivatives for $Z = 7$ with SF ($\alpha^* = 0.7,\ \zeta = 1.5,\ n = 7,\ l = 0$ and black color) and NSF ($\alpha^* = 1,\ \zeta = 1,\ n = 7,\ l = 0$ and red color) (color figure online)

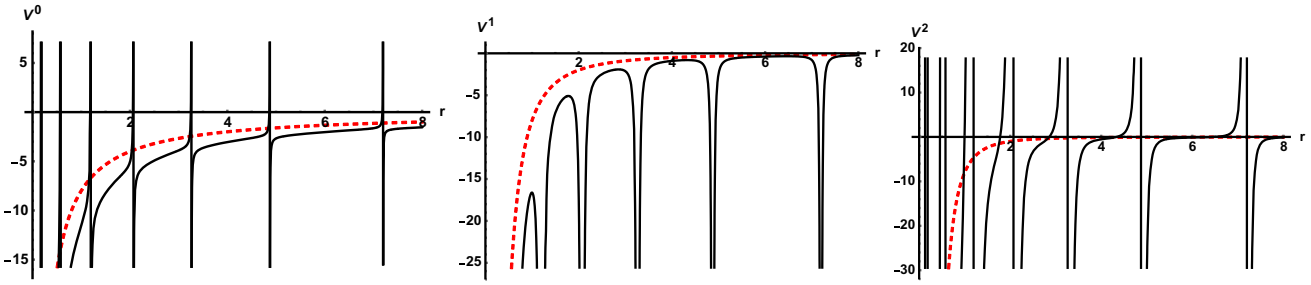

Fig. 8 Values of atomic anharmonic oscillator potential and its derivatives for $Z = 8$ with SF ($\alpha^* = 0.7,\ \zeta = 1.5,\ n = 8,\ l = 0$ and black color) and NSF ($\alpha^* = 1,\ \zeta = 1,\ n = 8,\ l = 0$ and red color) (color figure online)

4. Results and discussion

As can be seen from the suggested theory, the AAOPs and their derivatives are calculated with the help of formulae based on the use of the quantum nonperturbative theory in SF and NSF approximations. For the application, only the values of parameters n, l, α^* and ζ are required

By the use of the presented formulae, programs were constructed and performed in the Mathematica 7.0 software package. The calculations were performed on a Pentium Core at 2.5 GHz with 4 GB of RAM. The plots of the calculated NSF and SF potentials and their derivatives to versus radius vector for atomic particles are given in Figs. (1)–(8). The calculations are performed for the SP and NSF AAOPs and their derivatives for atomic particles $Z = 1$–8. The numerical results are obtained from an analytical formula for derivatives of the anharmonic oscillator, which enables one to calculate the SF force, force constant and others physical quantities. For the atomic particle for $Z = 2$, 4, 6 and 8 makes oscillations around the crucial points. It is seen from Figs. (1)–(8) that, in the case of $Z = 1$, 3, 5 and 7, the AAOPs take in the crucial points of the maximum number of infinite and minimal values. Similar calculations can be performed for $9 \leq Z < \infty$.

5. Conclusions

A new method is proposed for the evaluation of AAOPs and their derivatives using the quantum nonperturbative theory in SF and NSF approximations. It is that the quantum SF nonperturbative theory is efficient and promising for studies of AAOPs. Atomic units (a.u.) are used throughout.

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