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

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HIGHLIGHTS

- The physical nature of quantum self-frictional atomic potentials and nuclear attraction forces are presented.
- The quantum self-frictional potentials and nuclear attraction forces as a function of the distance from nucleus is analyzed.
- Model calculations have demonstrated high efficiency of the present approach.

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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) in standard convention, the self-frictional atomic potentials and nuclear attraction forces are investigated, where $p_l^* = 2l + 2 - \alpha^*$ and α^* is the integer ($\alpha^* = \alpha$, $-\infty < \alpha \leqslant 2$) or noninteger ($\alpha^* \neq \alpha$, $-\infty < \alpha^* < 3$) 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.

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. In the case of quantum self-frictional theory, first suggested by one of the author in the literature by extending Lorentz's damping theory, the electrons move around the atomic nuclei under two kinds of forces, namely, nuclear attraction and self-frictional forces. 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 [4–6], are the extensions of Lorentz theory to the quantum cases in standard convention (see Ref. [7] and references therein to our works on standard convention). 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 in standard convention is one of the greatest advances in modern physics.

We note that, in the case of disappearing self-frictional forces (for $\zeta = \frac{Z}{n}$ and $n = l + 1$), $\psi^{(p_l^*)}$-GETOs and eigenvalue are reduced to the Schrödinger's results in nonstandard convention which is common in quantum mechanics, where $\psi_{nlm}^{(1)} \equiv \psi_{nlm}$ is Schrödinger's noncomplete wave function. Since the Schrödinger's wave functions defined in Hilbert spaces are not complete sets, some convergence difficulties occur especially in series expansions. Accordingly, it is desirable to use the $\psi^{(p_l^*)}$-GETOs that are a large class (for

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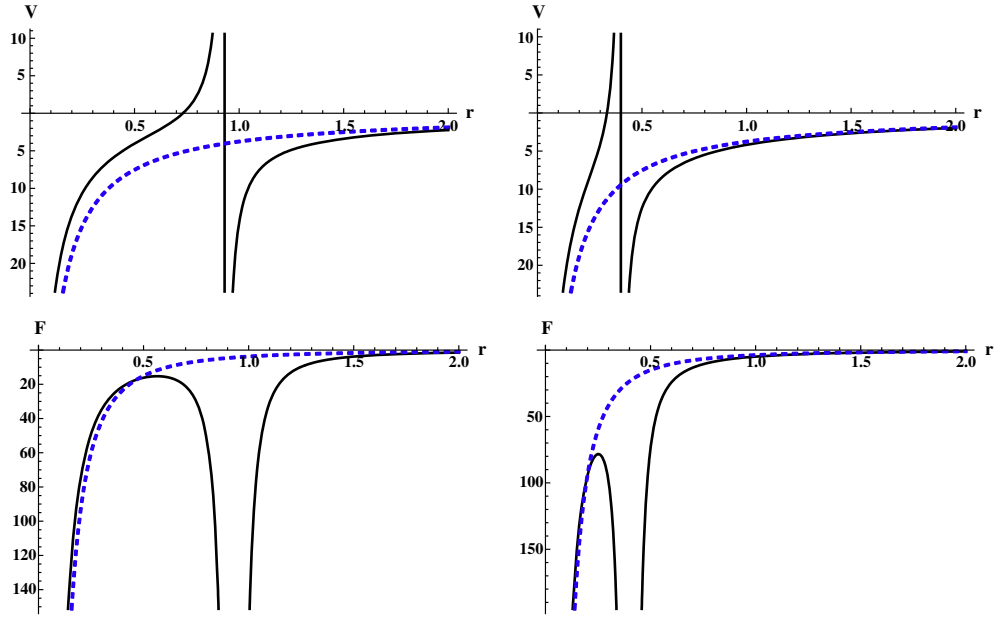

(a) $\alpha^*=-0.5$ (solid black lines) $\alpha^*=1$ (blue broken line)

(b) $\alpha^*=1.5$ (solid black lines) $\alpha^*=1$ (blue broken line)

Fig. 1. The self-frictional potentials and nuclear attraction forces as a function of distance from nucleus for $n=2$, $l=0$, $\zeta=1.88$ and $Y_{20}^{(p_l^*)}=1 (V\equiv V_{20}^{(p_l^*)}(\zeta,r); F\equiv F_{20}^{(p_l^*)}(\zeta,r))$.

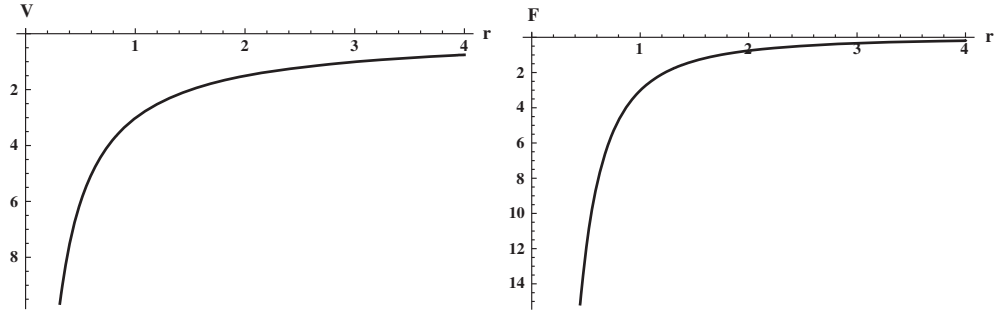

Fig. 2. The self-frictional potentials and nuclear attraction forces as a function of distance from nucleus for $n=2$, $l=1$, $\alpha^*=-0.5$, $\alpha^*=1.5$, $\zeta=1.51$ and $Y_{21}^{(p_l^*)}=0 (V\equiv V_{21}^{(p_l^*)}(\zeta,r); F\equiv F_{21}^{(p_l^*)}(\zeta,r))$.

$-\infty<\alpha^*<3$) of complete and orthonormal basis functions in corresponding Hilbert spaces.

The purpose of this work is, using formulas for $L^{(p_l^*)}$-GLPs and $\psi^{(p_l^*)}$-GETOs in standard convention, to construct the self-frictional atomic potentials and nuclear attraction forces for $1\leqslant n<\infty$, $0\leqslant l\leqslant n-1$, $-\infty<\alpha^*<3$ 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.

Theory

The atomic potentials and forces based on the use of $L^{(p_l^*)}$-GLPs in standard convention 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 [8],

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

The quantities $\left(-[q_n^*-p_l^*]\right)_k$ and $\left(p_l^*+1\right)_k$ in Eq. (6) are Pochhammer symbols [8].