

A PERTURBATIVE TREATMENT FOR THE ENERGY LEVELS OF NEUTRAL ATOMS

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Energy levels of neutral atoms have been reexamined by applying an alternative perturbative scheme in solving the Schrödinger equation for the Yukawa potential model with a modified screening parameter. The predicted shell binding energies are found to be quite accurate over the entire range of the atomic number Z up to 84 and compare very well with those obtained within the framework of hypervirial-Padé scheme and the method of shifted large- N expansion. It is observed that the new perturbative method may also be applied to the other areas of atomic physics.

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1. Introduction

In recent years the energy levels of neutral atoms have been studied by several analytic methods^{1–8} in which it is assumed that the screened potential of the atom may be of static screened Coulomb (SSC) which is well represented by Yukawa form:

$$V(r) = -\left(\frac{A}{r}\right) \exp(-\delta r), \quad (1)$$

with $A = \alpha Z e^2$, where $\alpha = (137.037)^{-1}$ is the fine-structure constant and Z is the atomic number. This form is often used for the description of the energy levels of light to heavy neutral atoms.⁷ It is known that SSC potential yields reasonable results only for the innermost states when Z is large. However, for the outermost and middle atomic states, it gives rather poor results. Although the bound state

energies for the SSC potential with $Z = 1$ have also been studied. The screening parameter δ is chosen to be

$$\delta = \delta_0 Z^{1/3}, \quad (2)$$

corresponding to the Z -dependence of the reciprocal of the Thomas–Fermi radius of the atom. However, these analytic works, perturbative as well as nonperturbative, fail to yield accurate shell binding energies for light atoms, particularly in the range $Z \leq 9$. Subsequently, it has been pointed out by Refs. 5 and 6 that the major source of errors perhaps lies in the wrong choice of the Z -dependence of the screening parameter. Invoking Fermi–Amaldi correction⁹ in the context of Ecker–Weizel approximation (EWA) method,¹⁰ Dutt and Varshni^{5–7} have suggested a modified form

$$\delta = \delta_0 Z^{1/3} \left(1 - \frac{1}{Z}\right)^{2/3}, \quad (3)$$

with $\delta_0 = 0.98$. Clearly, when $Z = 1$, δ vanishes and the potential in (1) becomes the Coulomb potential as it should be. Correctness of the choice of the modified screening parameter has been further justified by the recent work of Lai and Madan.⁸ They have shown that the hypervirial-Padé scheme which failed to reproduce correct shell binding energies for light atoms using the screening parameter given in (2),⁴ yields very accurate energy eigenvalues using the modified screening coefficient in (3).⁸ However, one of the shortcomings of the hypervirial-Padé technique is that it involves elaborate computational time and effort for each numerical prediction. Lai and Madan⁸ have to consider up to eleven terms in the perturbation series for the energy eigenvalues in order to ensure the convergence of the Padé approximant $E(N, M)$. Furthermore, application of this method becomes quite restricted due to nonavailability of compact analytic expressions for the bound-state energies, eigenfunctions and normalization constants.

On the other hand, Dutt and Varshni⁷ have investigated the bound-states of neutral atoms using the large- N expansion method which has been claimed to be very powerful for solving potential problems in nonrelativistic quantum mechanics. This technique also requires an approximate treatment and computational time as well.

In this paper, we investigate the bound-state properties of SSC potential using a new perturbative formalism^{11,12} which has been claimed to be very powerful for solving the Schrödinger equation to obtain the bound-state energies as well as the wave functions in Yukawa or SSC potential problem^{11–17} in both bound and continuum regions. This novel treatment is based on the decomposition of the radial Schrödinger equation into two pieces having an exactly solvable part with an additional piece leading to either a closed analytical solution or approximate treatment depending on the nature of the perturbed potential.

It seems then logical and meaningful to probe whether the range of applicability of this novel perturbation treatment may be widened. As a first attempt, we have

shown recently that the method adequately explains the spectrum of hydrogen-like atoms $A = Z = 1$ and also light and heavy atoms.^{18–20} With a view to make further applications to problems of atomic physics, we compute here the shell binding energies of light to heavy neutral atoms. The relevant steps of the perturbation scheme are to obtain analytical expressions for the bound-state energy levels and corresponding normalized eigenfunctions.

The contents of this paper is as follows. In Sec. 2 we briefly outline the method with all necessary formulae to perform the current calculations. In Sec. 3 we apply the approach to the Schrödinger equation with SSC potential and present the results obtained analytically and numerically for the bound-state energy values up to third perturbation energy shift. Finally, in Sec. 4 we give our concluding remarks.

2. The Method

For the consideration of spherically symmetric potentials, the corresponding Schrödinger equation, in the bound state domain, for the radial wave function reads

$$\frac{\hbar^2}{2m} \frac{\psi_n''(r)}{\psi_n(r)} = V(r) - E_n \tag{4}$$

with

$$V(r) = \left[V_0(r) + \frac{\hbar^2}{2m} \frac{\ell(\ell + 1)}{r^2} \right] + \Delta V(r), \tag{5}$$

where $\Delta V(r)$ is a perturbing potential and $\psi_n(r) = \chi_n(r)u_n(r)$ is the full radial wave function, in which $\chi_n(r)$ is the known normalized eigenfunction of the unperturbed Schrödinger equation whereas $u_n(r)$ is a moderating wave function corresponding to the perturbing potential. Following the prescription of Refs. 11–17, we may rewrite (4) in the form

$$\frac{\hbar^2}{2m} \left(\frac{\chi_n''(r)}{\chi_n(r)} + \frac{u_n''(r)}{u_n(r)} + 2 \frac{\chi_n'(r)u_n'(r)}{\chi_n(r)u_n(r)} \right) = V(r) - E_n. \tag{6}$$

The logarithmic derivatives of the unperturbed $\chi_n(r)$ and perturbed $u_n(r)$ wave functions are given by

$$W_n(r) = -\frac{\hbar}{\sqrt{2m}} \frac{\chi_n'(r)}{\chi_n(r)} \quad \text{and} \quad \Delta W_n = -\frac{\hbar}{\sqrt{2m}} \frac{u_n'(r)}{u_n(r)}, \tag{7}$$

which leads to

$$\frac{\hbar^2}{2m} \frac{\chi_n''(r)}{\chi_n(r)} = W_n^2(r) - \frac{\hbar}{\sqrt{2m}} W_n'(r) = \left[V_0(r) + \frac{\hbar^2}{2m} \frac{\ell(\ell + 1)}{r^2} \right] - \varepsilon_n, \tag{8}$$

where ε_n is the eigenvalue for the exactly solvable potential of interest, and

$$\begin{aligned} & \frac{\hbar^2}{2m} \left(\frac{u_n''(r)}{u_n(r)} + 2 \frac{\chi_n'(r)u_n'(r)}{\chi_n(r)u_n(r)} \right) \\ &= \Delta W_n^2(r) - \frac{\hbar}{\sqrt{2m}} \Delta W_n'(r) + 2W_n(r)\Delta W_n(r) = \Delta V(r) - \Delta\varepsilon_n, \end{aligned} \tag{9}$$

in which $\Delta\varepsilon_n = E_n^{(1)} + E_n^{(2)} + E_n^{(3)} + \dots$ is the correction term to the energy due to $\Delta V(r)$ and $E_n = \varepsilon_n + \Delta\varepsilon_n$. If Eq. (9), which is the most significant piece of the present formalism, can be solved analytically as in (8), then the whole problem, in Eq. (4) reduces to the following form:

$$[W_n(r) + \Delta W_n(r)]^2 - \frac{\hbar}{\sqrt{2m}}[W_n(r) + \Delta W_n(r)]' = V(r) - E_n, \tag{10}$$

which is a well-known treatment within the frame of supersymmetric quantum theory (SSQT).²¹ Thus, if the whole spectrum and corresponding eigenfunctions of the unperturbed interaction potential are known, then one can easily calculate the required superpotential $W_n(r)$ for any state of interest leading to direct computation of related corrections to the unperturbed energy and wave function.

For the perturbation technique, we can split the given potential in Eq. (4) into two parts. The main part corresponds to a shape invariant potential, Eq. (8), for which the superpotential is known analytically and the remaining part is treated as a perturbation, Eq. (9). Therefore, it is obvious that SSC potential can be treated using this prescription. In this regard, the zeroth-order term corresponds to the Coulomb potential while higher-order terms constitute the perturbation. However, the perturbation term in its present form cannot be solved exactly through Eq. (9). Thus, one should expand the functions related to the perturbation in terms of the perturbation parameter λ ,

$$\begin{aligned} \Delta V(r; \lambda) &= \sum_{i=1}^{\infty} \lambda_i V_i(r), \\ \Delta W_n(r; \lambda) &= \sum_{i=1}^{\infty} \lambda_i W_n^{(i)}(r), \\ E_n^{(i)}(\lambda) &= \sum_{i=1}^{\infty} \lambda_i E_n^{(i)}, \end{aligned} \tag{11}$$

where i denotes the perturbation order. Substitution of the above expansions into Eq. (9) and equating terms with the same power of λ on both sides up to $O(\lambda^4)$ gives

$$2W_n(r)W_n^{(1)}(r) - \frac{\hbar}{\sqrt{2m}} \frac{dW_n^{(1)}(r)}{dr} = V_1(r) - E_n^{(1)}, \tag{12}$$

$$W_n^{(1)}(r)W_n^{(1)}(r) + 2W_n(r)W_n^{(2)}(r) - \frac{\hbar}{\sqrt{2m}} \frac{dW_n^{(2)}(r)}{dr} = V_2(r) - E_n^{(2)}, \tag{13}$$

$$2[W_n(r)W_n^{(3)}(r) + W_n^{(1)}(r)W_n^{(2)}(r)] - \frac{\hbar}{\sqrt{2m}} \frac{dW_n^{(3)}(r)}{dr} = V_3(r) - E_n^{(3)}, \tag{14}$$

$$2[W_n(r)W_n^{(4)}(r) + W_n^{(1)}(r)W_n^{(3)}(r)] + W_n^{(2)}(r)W_n^{(2)}(r) - \frac{\hbar}{\sqrt{2m}} \frac{dW_n^{(4)}(r)}{dr} = V_4(r) - E_n^{(4)}. \tag{15}$$

Hence, unlike the other perturbation theories, Eq. (9) and its expansion, Eqs. (12)–(15), give a flexibility for the easy calculations of the perturbative corrections to energy and wave functions for the n th state of interest through an appropriately chosen perturbed superpotential.

3. Application to the SSC Potential

Considering the recent interest in various power-law potentials in the literature, we work through the paper within the frame of low screening parameter. In this case, the SSC or Yukawa potential can be expanded in power series of the screening parameter δ as²²

$$V(r) = -\left(\frac{A}{r}\right) \exp(-\delta r) = -\left(\frac{A}{r}\right) \sum_{i=0}^{\infty} V_i(\delta r)^i, \tag{16}$$

where the perturbation coefficients V_i are given by

$$V_1 = -1, \quad V_2 = 1/2, \quad V_3 = -1/6, \quad V_4 = 1/24, \dots \tag{17}$$

We now apply this approximation method to Yukawa potential with the angular momentum barrier

$$V(r) = -\left(\frac{A}{r}\right) \exp(-\delta r) + \frac{\ell(\ell + 1)\hbar^2}{2mr^2} = \left[V_0(r) + \frac{\ell(\ell + 1)\hbar^2}{2mr^2} \right] + \Delta V(r), \tag{18}$$

where the first piece is the shape invariant zeroth-order which is an exactly solvable piece corresponding to the unperturbed Coulomb potential with $V_0(r) = -A/r$ while $\Delta V(r) = A\delta - (A\delta^2/2)r + (A\delta^3/6)r^2 - (A\delta^4/24)r^3 + \dots$ is the perturbation term. The literature is rich with examples of particular solutions for such power-law potentials employed in different fields of physics, for recent applications see Refs. 23 and 24. At this stage one may wonder why the series expansion is truncated at a lower order. This can be understood as follows. It is widely appreciated that convergence is not an important or even desirable property for series approximations in physical problems. Specifically, a slowly convergent approximation which requires many terms to achieve reasonable accuracy is much less valuable than the divergent series which gives accurate answers in a few terms. This is clearly the case for the Yukawa problem.²⁵ However, it is worthwhile to note that the main contributions come from the first four terms. Thereby, the present calculations are performed up to the third order involving only these additional potential terms, which surprisingly provide highly accurate results for small screening parameter δ .

3.1. Ground state calculations ($n = 0$)

In the light of Eq. (8), the zeroth-order calculations leading to exact solutions can be carried out readily by setting the ground-state superpotential and the unperturbed exact energy as

$$\begin{aligned}
 W_{n=0}(r) &= -\frac{\hbar}{\sqrt{2m}} \frac{\ell + 1}{r} + \sqrt{\frac{m}{2}} \frac{A}{(\ell + 1)\hbar}, \\
 E_n^{(0)} &= -\frac{mA^2}{2\hbar^2(n + \ell + 1)^2}, \quad n = 0, 1, 2, \dots
 \end{aligned}
 \tag{19}$$

and from the literature, the corresponding normalized Coulomb bound-state wave function²⁶

$$\chi_n^{(C)}(r) = N_{n,l}^{(C)} r^{\ell+1} \exp[-\beta r] \times L_n^{2\ell+1}[2\beta r],
 \tag{20}$$

in which $N_{n,l}^{(C)} = \left[\frac{2mA}{(n+\ell+1)\hbar^2} \right]^{\ell+1} \frac{1}{(n+\ell+1)} \frac{1}{\sqrt{\frac{\hbar^2}{mA n!} (n+2\ell+1)!}}$ is a normalized constant, $\beta = \frac{mA}{(n+\ell+1)\hbar^2}$ and $L_n^k(x) = \sum_{m=0}^n (-1)^m \frac{(n+k)!}{(n-m)!(m+k)!m!} x^m$ is an associate Laguerre polynomial function.²⁷

For the sake of calculation of corrections to the zeroth-order energy and wave function, one needs to consider the expressions leading to the first- and third-order perturbation given by Eqs. (12)–(15). Multiplication of each term in these equations by $\chi_n^2(r)$, and bearing in mind the superpotentials given in Eq. (7), one can obtain the straightforward expressions for the first-order correction to the energy and its superpotential:

$$\begin{aligned}
 E_n^{(1)} &= \int_{-\infty}^{\infty} \chi_n^2(r) \left(-\frac{A\delta^2}{2} r \right) dr, \\
 W_n^{(1)}(r) &= \frac{\sqrt{2m}}{\hbar} \frac{1}{X_n^2(r)} \int^r \chi_n^2(x) \left[E_n^{(1)} + \frac{A\delta^2}{2} x \right] dx,
 \end{aligned}
 \tag{21}$$

and for the second-order correction and its superpotential:

$$\begin{aligned}
 E_n^{(2)} &= \int_{-\infty}^{\infty} \chi_n^2(r) \left[\frac{A\delta^3}{6} r^2 - W_n^{(1)}(r)W_n^{(1)}(r) \right] dr, \\
 W_n^{(2)}(r) &= \frac{\sqrt{2m}}{\hbar} \frac{1}{X_n^2(r)} \int^r \chi_n^2(x) \left[E_n^{(2)} + W_n^{(1)}(x)W_n^{(1)}(x) - \frac{A\delta^3}{6} x^2 \right] dx,
 \end{aligned}
 \tag{22}$$

and for the third-order correction and its superpotential:

$$\begin{aligned}
 E_n^{(3)} &= \int_{-\infty}^{\infty} \chi_n^2(r) \left[-\frac{A\delta^4}{24} r^3 - W_n^{(1)}(r)W_n^{(2)}(r) \right] dr, \\
 W_n^{(3)}(r) &= \frac{\sqrt{2m}}{\hbar} \frac{1}{X_n^2(r)} \int^r \chi_n^2(x) \left[E_n^{(3)} + W_n^{(1)}(x)W_n^{(2)}(x) + \frac{A\delta^4}{24} x^3 \right] dx,
 \end{aligned}
 \tag{23}$$

for any state of interest. The above expressions calculate $W_n^{(1)}(r)$, $W_n^{(2)}(r)$ and $W_n^{(3)}(r)$ explicitly from the energy corrections $E_n^{(1)}$, $E_n^{(2)}$ and $E_n^{(3)}$ respectively, which are in turn used to calculate the moderating wave function $u_n(r)$.

Thus, through the use of Eqs. (21)–(23), one finds the ground state energy shift up to the third order and their moderating superpotentials as

$$\begin{aligned}
 E_0^{(1)} &= -\frac{\hbar^2(3N_0^2 - L)}{4m} \delta^2, \\
 E_0^{(2)} &= \frac{\hbar^4 N_0^2(5N_0^2 - 3L + 1)}{12Am^2} \delta^3 - \frac{\hbar^6 N_0^4(5N_0^2 - 3L + 1)}{16A^2m^3} \delta^4, \\
 E_0^{(3)} &= -\frac{\hbar^6 N_0^2(5N_0^2 - 3L)(5N_0^2 - 3L + 1)}{96A^2m^3} \delta^4 \\
 &\quad + \frac{\hbar^8 N_0^4(5N_0^2 - 3L + 1)(9N_0^2 - 5L)}{48A^3m^4} \delta^5 \\
 &\quad - \frac{\hbar^{10} N_0^6(5N_0^2 - 3L + 1)(9N_0^2 - 5L)}{64A^4m^5} \delta^6, \\
 W_0^{(1)}(r) &= -\frac{\hbar N_0 \delta^2}{2\sqrt{2m}} r, \\
 W_0^{(2)}(r) &= -\frac{\hbar N_0 [Amr + \hbar^2 N_0 N_1] [3\hbar^2 N_0^2 \delta - 4mA] \delta^3}{24\sqrt{2m}(Am)^2} r,
 \end{aligned} \tag{24}$$

where $N_0 = (\ell + 1)$, $N_1 = (\ell + 2)$ and $L = \ell(\ell + 1)$. Therefore, the analytical expressions for the lowest energy and full radial wave function of the Yukawa potential are then given by

$$\begin{aligned}
 E_{n=0,\ell} &= E_{n=0}^{(0)} + A\delta + E_0^{(1)} + E_0^{(2)} + E_0^{(3)} + \dots, \\
 \psi_{n=0,\ell}(r) &\approx \chi_{n=0,\ell}^{(C)}(r) u_{n=0,\ell}(r),
 \end{aligned} \tag{25}$$

in which

$$u_{n=0,\ell}(r) \approx \exp\left(-\frac{\sqrt{2m}}{\hbar} \int^r (W_0^{(1)}(x) + W_0^{(2)}(x)) dx\right). \tag{26}$$

Hence, the explicit form of the full wave function in (25) for the ground state is

$$\psi_{n=0,\ell}(r) = \left[\frac{2mA}{(\ell + 1)\hbar^2}\right]^{\ell+1} \frac{1}{(\ell + 1)} \sqrt{\frac{Am}{\hbar^2(2\ell + 1)!}} r^{\ell+1} \exp(P(r)), \tag{27}$$

with $P(r) = \sum_{i=2}^3 p_i r^i$ is a polynomial of third order having the following coefficients:

$$p_2 = b \left[1 + \frac{\hbar^2 N_0 N_1 c}{Am}\right], \quad p_3 = \frac{2}{3} bc, \tag{28}$$

in which

$$b = \frac{1}{4} N_0 \delta^2, \quad c = \frac{\delta}{12Am} [3\hbar^2 N_0^2 \delta - 4Am]. \tag{29}$$

3.2. Excited state calculations ($n \geq 1$)

The calculations procedures lead to a handy recursion relations in the case of ground states, but becomes extremely cumbersome in the description of radial excitations when nodes of wave functions are taken into account, in particular during the higher order calculations. Although several attempts have been made to bypass this difficulty and improve calculations in dealing with excited states, (cf. e.g. Ref. 28, and the references therein) within the frame of supersymmetric quantum mechanics (SUSYQM).

Using Eqs. (7) and (19), the superpotential $W_n(r)$ which is related to the excited states can be readily calculated through Eqs. (21)–(23). So the first-order energy shift in the first excited state ($n = 1$) and its superpotential are

$$E_1^{(1)} = -\frac{\hbar^2(3N_1^2 - L)}{4m}\delta^2, \quad W_1^{(1)}(r) \approx -\frac{\hbar N_1 \delta^2}{2\sqrt{2m}}r. \tag{30}$$

Consequently, the use of the approximated $W_1^{(1)}(r)$ in the preceeding equation in (22) gives the energy correction in the second order as

$$E_1^{(2)} = \frac{\hbar^4 N_1^2(5N_1^2 - 3L + 1)}{12Am^2}\delta^3 - \frac{\hbar^6 N_1^4(5N_1^2 - 3L + 1)}{16A^2m^3}\delta^4. \tag{31}$$

We also find its supersymmetric potential

$$W_1^{(2)}(r) = -\frac{\hbar N_1[Amr + \hbar^2 N_1 N_2][3\hbar^2 N_1^2 \delta - 4mA]\delta^3}{24\sqrt{2m}(Am)^2}r, \tag{32}$$

which gives the energy shift in the third order as

$$\begin{aligned} E_1^{(3)} = & -\frac{\hbar^6 N_1^2(5N_1^2 - 3L)(5N_1^2 - 3L + 1)}{96A^2m^3}\delta^4 \\ & + \frac{\hbar^8 N_1^4(5N_1^2 - 3L + 1)(9N_1^2 - 5L)}{48A^3m^4}\delta^5 \\ & - \frac{\hbar^{10} N_1^6(5N_1^2 - 3L + 1)(9N_1^2 - 5L)}{64A^4m^5}\delta^6. \end{aligned} \tag{33}$$

Therefore, the approximated energy value of the Yukawa potential corresponding to the first excited state is

$$E_{n=1,\ell} = E_1^{(0)} + A\delta + E_1^{(1)} + E_1^{(2)} + E_1^{(3)} + \dots. \tag{34}$$

The related radial wave function can be expressed in an analytical form in the light of Eqs. (21)–(23) and Eq. (25), if required. The approximation used in this work would not affect considerably the sensitivity of the calculations. On the other hand, it is found analytically that our investigations put forward an interesting hierarchy between $W_n^{(1)}(r)$ terms of different quantum states in the first order after circumventing the nodal difficulties elegantly,

$$W_n^{(1)}(r) \approx -\frac{\hbar(n + \ell + 1)\delta^2}{2\sqrt{2m}}r, \tag{35}$$

which, for instance, for the second excited state ($n = 2$) leads to the first-order correction

$$E_2^{(1)} = -\frac{\hbar^2(3N_2^2 - L)}{4m}\delta^2, \quad W_2^{(1)}(r) \approx -\frac{\hbar N_2\delta^2}{2\sqrt{2m}}r. \quad (36)$$

Thus, the use of the approximated $W_2^{(1)}(r)$ in the preceding equation (22) gives the energy shift in the second order and its superpotential as

$$E_2^{(2)} = \frac{\hbar^4 N_2^2(5N_2^2 - 3L + 1)}{12Am^2}\delta^3 - \frac{\hbar^6 N_2^4(5N_2^2 - 3L + 1)}{16A^2m^3}\delta^4, \quad (37)$$

$$W_2^{(2)}(r) = -\frac{\hbar N_2[Amr + \hbar^2 N_2 N_3][3\hbar^2 N_2^2\delta - 4mA]\delta^3}{24\sqrt{2m}(Am)^2}r,$$

which leads, via Eq. (23), into the third-order energy shift

$$E_2^{(3)} = -\frac{\hbar^6 N_2^2(5N_2^2 - 3L)(5N_2^2 - 3L + 1)}{96A^2m^3}\delta^4$$

$$+ \frac{\hbar^8 N_2^4(5N_2^2 - 3L + 1)(9N_2^2 - 5L)}{48A^3m^4}\delta^5$$

$$- \frac{\hbar^{10} N_2^6(5N_2^2 - 3L + 1)(9N_2^2 - 5L)}{64A^4m^5}\delta^6, \quad (38)$$

where $N_2 = (\ell + 3)$. Therefore, the approximated energy eigenvalue of the Yukawa potential corresponding to the second excited state ($n = 2$) is

$$E_{n=2,\ell} = E_2^{(0)} + A\delta + E_2^{(1)} + E_2^{(2)} + E_2^{(3)} + \dots. \quad (39)$$

Finally, from the supersymmetry, we find out the n th-state energy shifts together with their supersymmetric potentials as

$$E_n^{(1)} = -\frac{\hbar^2[3(n+l+1)^2 - L]}{4m}\delta^2,$$

$$W_n^{(1)}(r) \approx -\frac{\hbar(n+l+1)\delta^2}{2\sqrt{2m}}r,$$

$$E_n^{(2)} = \frac{\hbar^4(n+l+1)^2[5(n+l+1)^2 - 3L + 1]}{12Am^2}\delta^3$$

$$- \frac{\hbar^6(n+l+1)^4[5(n+l+1)^2 - 3L + 1]}{16A^2m^3}\delta^4, \quad (40)$$

$$W_n^{(2)}(r) = -\frac{\hbar^4(n+l+1)[Amr + \hbar^2(n+l+1)(n+l+2)][3\hbar^2(n+l+1)^2\delta - 4mA]\delta^3}{24\sqrt{2m}(Am)^2}r,$$

$$E_n^{(3)} = -\frac{\hbar^6(n+l+1)^2[5(n+l+1)^2 - 3L][5(n+l+1)^2 - 3L + 1]}{96A^2m^3}\delta^4$$

$$+ \frac{\hbar^8(n+l+1)^4[5(n+l+1)^2 - 3L + 1][9(n+l+1)^2 - 5L]}{48A^3m^4}\delta^5$$

$$- \frac{\hbar^{10}(n+l+1)^6[5(n+l+1)^2 - 3L + 1][9(n+l+1)^2 - 5L]}{64A^4m^5}\delta^6.$$

Table 1. Calculated K -shell energies E_{00} in keV for some values of Z .

Z	EWA (Ref. 5)	Hypervirial-Padé (Ref. 8)	Shifted- N (Ref. 7)	Expt. (Ref. 29)	Present work
3	-0.053 34	-0.054 15	-0.054 14	-0.054 75	-0.054 056 87
4	-0.105	-0.106 34	-0.106 34	-0.111	-0.106 281 60
5	-0.178	-0.180 08	-0.180 07	-0.188	-0.180 078 08
6	-0.274	-0.276 23	-0.276 23	-0.284	-0.276 306 26
7	-0.393	-0.395 42	-0.395 41	-0.402	-0.395 579 11
8	-0.535	-0.538 09	-0.538 09	-0.532	-0.538 354
9	-0.701	-0.704 61	-0.704 61	-0.685	-0.704 983
14	-1.897	-1.903 20	-1.903 20	-1.839	-1.904 306
19	-3.716	-3.725 45	-3.725 45	-3.607	-3.727 639
24	-6.171	-6.182 77	-6.182 77	-5.989	-6.186 408
29	-9.268	-9.282 12	-9.282 13	-8.979	-9.287 593
34	-13.012	-13.028 30	-13.028 30	-12.658	-13.035 977
39	-17.407	-17.424 82	-17.424 82	-17.038	-17.435 077
44	-22.454	-22.474 38	-22.474 38	-22.117	-22.487 609
49	-28.157	-28.179 15	-28.179 15	-27.940	-28.195 740
54	-34.517	-34.540 92	-34.540 92	-34.561	-34.561 250
59	-41.535	-41.566 12	-41.561 17	-41.991	-41.585 000
64	-49.213	-49.241 18	-49.241 18	-50.239	-49.270 154
69	-57.553	-57.582 03	-57.582 03	-59.390	-57.615 917
74	-66.554	-66.584 70	-66.584 70	-69.525	-66.623 882
79	-76.217	-76.250 03	-76.250 03	-80.725	-76.294 897
84	-86.544	-86.578 78	-86.578 78	-93.105	-86.629 718

Thus, the total energy for the n th state is

$$E_{n,\ell} = E_n^{(0)} + A\delta + E_n^{(1)} + E_n^{(2)} + E_n^{(3)} + \dots \quad (41)$$

For the numerical results, in Tables 1–3, we list our calculated K - and L -shell binding energies for some values of Z and compare those with the hypervirial-Padé results,⁸ the shifted large- N expansion method⁷ and the experimental values²⁹ for the s -state energies E_{00} and E_{10} and also the p -state energies E_{01} and E_{11} . It is observed that inspite of calculational simplicity, the present approach yields results as accurate as predicted by more elaborate hypervirial-Padé and shifted large- N expansion calculation. Finally, the scope of extending the method to calculate oscillator strength, bound-bound transition matrix elements etc. which have significant importance in atomic physics is also possible.

4. Concluding Remarks

In Tables 1–3 we present our calculated K -shell binding energies E_{00} and E_{01} and L -shell binding energies E_{10} and E_{11} for some values of Z and compare them with the predictions of Lai and Madan⁸ and the experimental values.²⁴ We quote only the Padé approximant^{10,11} E results which provide upper bound to the energy eigenvalues for E_{10} and E_{20} levels. We also depict our earlier results⁵ obtained through EWA method which provides compact analytic expressions only for the

Table 2. Calculated K -shell energies E_{01} in keV for some values of Z .

Z	E_{01}	Z	E_{01}
9	-0.012 158	49	-4.207 958
14	-0.089 499	54	-5.358 162
19	-0.282 475	59	-6.655 877
24	-0.598 417	64	-8.102 492
29	-1.044 023	69	-9.699 206
34	-1.624 349	74	-11.447 062
39	-2.343 224	79	-13.346 979
44	-3.203 631	84	-15.399 774

Table 3. Calculated L -shell energies E_{10} in keV for some values of Z .

Z	EWA (Ref. 5)	Hypervirial-Padé (Ref. 8)	Shifted- N (Ref. 7)	Expt. (Ref. 29)	Present work
9	-0.018	-0.022 06	-0.026 30	-0.031	-0.042 259
14	-0.116	-0.124 92	-0.124 92	-0.149	-0.130 396
19	-0.320	-0.335 03	-0.335 03	-0.377	-0.338 344
24	-0.644	-0.665 54	-0.665 54	-0.695	-0.669 125
29	1.096	-1.124 48	-1.124 48	-1.096	-1.128 848
34	-1.692	-1.717 35	-1.717 35	-1.654	-1.722 569
39	-2.407	-2.448 16	-2.450 36	-2.373	-2.454 212
44	-3.272	-3.319 98	-3.322 03	-3.224	-3.326 856
49	-4.281	-4.335 27	-4.337 19	-4.238	-4.342 964
54	-5.435	-5.496 02	-5.497 83	-5.453	-5.504 555
59	-6.737	-6.803 90	-6.805 63	-6.835	-6.813 316
64	-8.187	-8.260 34	-8.261 99	-8.376	-8.270 675
69	-9.787	-9.866 54	-9.868 12	-10.116	-9.877 861
74	-11.538	-11.623 58	-11.625 10	-12.100	-11.635 946
79	-13.441	-13.532 38	-13.533 85	-14.353	-13.545 871
84	-15.496	-15.593 79	-15.595 21	-16.939	-15.608 473

bound s -state energy eigenvalues. As we have used throughout the atomic units, our energies are measured in units of $2 Ry = 27.212$ eV is used.²⁵ One may notice that in comparison to our earlier calculation based on EWA method, the present techniques gives much improved energy eigenvalues. Furthermore, our predictions are surprisingly close to those obtained through the use of elaborate hypervirial technique. This indicates that there is distinct advantage in using the shifted large- N method to similar calculations as it yields very accurate results yet remaining simple and straightforward.

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