Energy levels of neutral atoms via a new perturbation method

Omar Mustafa† and Maen Odeh‡
Department of Physics, Eastern Mediterranean University
G. Magusa, North Cyprus, Mersin 10 - Turkey
† omar.mustafa@mozart.emu.edu.tr
‡ odeh.as@mozart.emu.edu.tr

Abstract

The energy levels of neutral atoms supported by Yukawa potential, \( V(r) = -Z \exp(-ar)/r \), are studied, using both dimensional and dimensionless quantities, via a new analytical methodical proposal (devised to solve for nonexactly solvable Schrödinger equation). Using dimensionless quantities, by scaling the radial Hamiltonian through \( y = Zr \) and \( \alpha' = a/Z \), we report that the scaled screening parameter \( \alpha' \) is restricted to have values ranging from zero to less than 0.4. On the other hand, working with the scaled Hamiltonian enhances the accuracy and extremely speeds up the convergence of the energy eigenvalues. The energy levels of several new eligible scaled screening parameter \( \alpha' \) values are also reported.
1 Introduction

The Yukawa potential plays special roles in different branches of physics. It is known as the Debye-Hückel potential in plasma physics, as the Thomas-Fermi or screened Coulomb potential in solid-state and atomic physics, and the Yukawa potential in nuclear physics. It is also used in the models describing metal-insulator transition [1,2]. As such, several approaches have been invested to find the energy levels of this potential. Amongst exist the simple variational procedure [3], the use of atomic orbitals with a set of fitting parameters [4], Rayleigh-Schrödinger perturbation theory [5,6], method of potential envelopes [7], iterative procedure [8], different numerical calculations [9,10], and the shifted 1/N expansion method [11] based on Papp’s [12] or Imbo et al.’s [13,14] proposals.

On the other hand, the Yukawa form

\[ V(r) = -Z\exp(-\alpha r)/r \]

is known to simulate the screening potential of neutral atoms, where the screening parameter \( \alpha \) is chosen to be \( \alpha = \alpha_o Z^{1/3} \) corresponding to the \( Z \)-dependence of the reciprocal of the Thomas-Fermi radius of the atom. However, invoking Fermi-Amaldi correction [15] in the context of Ecker-Weizel approximation (EWA) method [16], Dutt and Varshni [17] have amended the screening parameter and suggested that \( \alpha = \alpha_o Z^{1/3}(1 - 1/Z)^{2/3} \) with \( \alpha_o = 0.98 \). The correctness of this amendment has been justified by Lai and Madan [18], who have used the hypervirial-Padé method (HPM) to obtain very accurate energy eigenvalues. Therefore, the energy levels of the neutral atoms, supported by potential (1), have been reexamined by applying the shifted large-N expansion (SLNT) (where \( N \) is the number of spatial dimensions) [14]. However, some drawbacks of the HPM and SLNT are in order. The HPM involves elaborate computational time and effort for each numerical prediction, and its application becomes quite restricted due to the absence of compact analytical expressions for the eigenenergies and eigenfunctions. And, because of the complexity in handling large-order corrections of the standard Rayleigh-Schrödinger perturbation theory, only low-order eigenenergy calculations have been reported for SLNT and large order-calculations have been neglected [11-14]. Yet, nei-
ther SLNT nor HPM is utilitarian in terms of calculating the eigenvalues and eigenfunctions in one batch. Moreover, Scherrer et al. [19] have concluded, via matrix continued fractions method, that SLNT leads to dubious accuracies. A conclusion that we have very recently confirmed [20].

In this work we introduce a new methodical proposal for solving Schrödinger equation with an arbitrary spherically symmetric potential. We shall use $1/\bar{l}$ as an expansion parameter, where $\bar{l} = l - \beta$, $l$ is a quantum number and $\beta$ a suitable shift introduced, mainly, to avoid the trivial case $l = 0$. In fact, the scope of its applicability is not limited to the spherically symmetric problems, it extends also to systems at lower dimensions. Here is the conversion strategy. One would rewrite the centrifugal term $l(l + 1)/2r^2$, in Eq.(2) below, as $\Lambda(\Lambda + 1)/(2q^2)$ and use $1/\bar{\Lambda}$ as an expansion parameter. In this case, $\Lambda = l$ in three dimensions, where $l$ is the angular momentum quantum number with $q = r > 0$, $\Lambda = |m| - 1/2$ in two dimensions, where $m$ is the magnetic quantum number with $q = (x^2 + y^2)^{1/2} > 0$, and $\Lambda = -1$ and/or $0$ in one dimension with $-\infty < q < \infty$. Thus the method could be called a pseudoperturbative shifted - $l$ expansion technique (PSLET), to be described in the following section.

2 The Method

To construct the method we start with the time - independent one - dimensional form of Schrödinger equation, in $\hbar = m = 1$ units,

$$\left[ -\frac{1}{2} \frac{d^2}{dr^2} + \frac{l(l + 1)}{2r^2} + V(r) \right] \Psi_{n,r,l}(r) = E_{n,r,l} \Psi_{n,r,l}(r). \quad (2)$$

and to avoid the trivial case $l=0$, the quantum number $l$ is shifted through the relation $\bar{l} = l - \beta$. Eq.(2) thus becomes

$$\left\{ -\frac{1}{2} \frac{d^2}{dr^2} + \bar{V}(r) \right\} \Psi_{n,r,l}(r) = E_{n,r,l} \Psi_{n,r,l}(r), \quad (3)$$

$$\bar{V}(r) = \frac{\bar{l}^2 + (2\beta + 1)\bar{l} + \beta(\beta + 1)}{2r^2} + \frac{\bar{l}^2}{Q} V(r). \quad (4)$$
Herein, it should be noted that $Q$ is a constant that scales the potential $V(r)$ at large - $l$ limit and is set, for any specific choice of $l$ and $n_r$, equal to $l^2$ at the end of the calculations [11-14,20-22]. And, $\beta$ is to be determined in the sequel.

Our systematic procedure begins with shifting the origin of the coordinate through

$$x = \tilde{r}^{1/2}(r - r_0)/r_0, \quad (5)$$

where $r_0$ is currently an arbitrary point to perform Taylor expansions about, with its particular value to be determined. Expansions about this point, $x = 0$ (i.e. $r = r_0$), yield

$$\frac{1}{r^2} = \sum_{n=0}^{\infty} (-1)^n \frac{(n+1)}{r_0^n} x^n \tilde{r}^{-n/2}, \quad (6)$$

$$V(x(r)) = \sum_{n=0}^{\infty} \left( \frac{d^n V(r_0)}{dr_0^n} \right) \frac{(r_0 x)^n}{n!} \tilde{r}^{-n/2}. \quad (7)$$

Obviously, the expansions in (6) and (7) center the problem at an arbitrary point $r_0$ and the derivatives, in effect, contain information not only at $r_0$ but also at any point on the axis, in accordance with Taylor’s theorem. Also, it should be mentioned here that the scaled coordinate, equation (5), has no effect on the energy eigenvalues, which are coordinate - independent. It just facilitates the calculations of both the energy eigenvalues and eigenfunctions. It is also convenient to expand $E$ as

$$E_{n_r,l} = \sum_{n=0}^{\infty} E_{n_r,l}^{(n)} \tilde{r}^{-n}. \quad (8)$$

Equation (3) thus becomes

$$\left[ -\frac{1}{2} \frac{d^2}{dx^2} + \frac{r_0^2}{l} V(x(r)) \right] \Psi_{n_r,l}(x) = \frac{r_0^2}{l} E_{n_r,l} \Psi_{n_r,l}(x), \quad (9)$$
where the prime of $V(r_0)$ denotes derivative with respect to $r_0$. Equation (9) is exactly of the type of Schrödinger equation for one-dimensional anharmonic oscillator

$$\left[-\frac{1}{2} \frac{d^2}{dx^2} + \frac{1}{2} w^2 x^2 + \varepsilon_0 + P(x)\right] X_{n,r}(x) = \lambda_{n,r} X_{n,r}(x),$$

(11)

where $P(x)$ is a perturbation-like term and $\varepsilon_0$ is a constant. A simple comparison between Eqs.(9), (10) and (11) implies

$$\varepsilon_0 = \bar{l} \left[\frac{1}{2} + \frac{r_0^2 V(r_0)}{Q}\right] + \frac{2\beta + 1}{2} + \frac{\beta(\beta + 1)}{2\bar{l}},$$

(12)

$$\lambda_{n,r} = \bar{l} \left[\frac{1}{2} + \frac{r_0^2 V(r_0)}{Q}\right] + \frac{2\beta + 1}{2} + \frac{(n_r + 1/2)w}{n_r} + \sum_{n=2}^{\infty} \lambda_{n,r}^{(n-1)} \bar{l}^{-n},$$

(13)

and

$$\lambda_{n,r} = r_0^2 \sum_{n=-2}^{\infty} E_{n,r}^{(n)} \bar{l}^{-(n+1)},$$

(14)
Equations (13) and (14) yield

\[ E_{n_r,l}^{(-2)} = \frac{1}{2r_0^2} + \frac{V(r_0)}{Q} \]  

(15)

\[ E_{n_r,l}^{(-1)} = \frac{1}{r_0^2} \left[ \frac{2\beta + 1}{2} + (n_r + \frac{1}{2})w \right] \]  

(16)

\[ E_{n_r,l}^{(0)} = \frac{1}{r_0^2} \left[ \frac{\beta(\beta + 1)}{2} + \lambda_{n_r}^{(0)} \right] \]  

(17)

\[ E_{n_r,l}^{(n)} = \lambda_{n_r}^{(n)}/r_0^2 ; \quad n \geq 1. \]  

(18)

Here \( r_0 \) is chosen to minimize \( E_{n_r,l}^{(-2)} \), i.e.

\[ \frac{dE_{n_r,l}^{(-2)}}{dr_0} = 0 \quad \text{and} \quad \frac{d^2E_{n_r,l}^{(-2)}}{dr_0^2} > 0. \]  

(19)

Hereby, \( V(r) \) is assumed to be well behaved so that \( E^{(-2)} \) has a minimum \( r_0 \) and there are well-defined bound-states. Equation (19) in turn gives, with \( \bar{l} = \sqrt{Q} \),

\[ l - \beta = \sqrt{r_0^3V'(r_0)}. \]  

(20)

Consequently, the second term in Eq.(10) vanishes and the first term adds a constant to the energy eigenvalues. It should be noted that energy term \( \bar{l}^2E_{n_r,l}^{(-2)} \) has its counterpart in classical mechanics. It corresponds roughly to the energy of a classical particle with angular momentum \( L_z = \bar{l} \) executing circular motion of radius \( r_0 \) in the potential \( V(r_0) \). This term thus identifies the leading-order approximation, to all eigenvalues, as a classical approximation and the higher-order corrections as quantum fluctuations around the minimum \( r_0 \), organized in inverse powers of \( \bar{l} \).
The next leading correction to the energy series, $\tilde{E}^{(-1)}_{n_r,l}$, consists of a constant term and the exact eigenvalues of the unperturbed harmonic oscillator potential $w^2x^2/2$. The shifting parameter $\beta$ is determined by choosing $\tilde{E}^{(-1)}_{n_r,l}=0$. This choice is physically motivated. It requires not only the agreements between PSLET eigenvalues and the exact known ones for the harmonic oscillator and Coulomb potentials but also between the eigenfunctions as well. Hence

$$\beta = -\left[\frac{1}{2} + (n_r + \frac{1}{2})w\right],$$

where

$$w = \sqrt{3 + \frac{r_0V''(r_0)}{V'(r_0)}}.$$ (22)

Then equation (10) reduces to

$$\frac{r_0^2}{l}\tilde{V}(x(r)) = r_0^2\tilde{l}\left[\frac{1}{2r_0^2} + \frac{V(r_0)}{Q}\right] + \sum_{n=0}^{\infty} v^{(n)}(x)\tilde{l}^{-n/2},$$ (23)

where

$$v^{(0)}(x) = \frac{1}{2}w^2x^2 + \frac{2\beta + 1}{2},$$ (24)

$$v^{(1)}(x) = -(2\beta + 1)x - 2x^3 + \frac{r_0^2V'''(r_0)}{6Q}x^3,$$ (25)

and for $n \geq 2$

$$v^{(n)}(x) = (-1)^n(2\beta + 1)\frac{(n+1)}{2}x^n + (-1)^n\frac{\beta(\beta + 1)}{2}(n-1)x^{(n-2)}$$

$$+ \left[(-1)^n\frac{(n+3)}{2} + \frac{r_0^{(n+4)}}{Q(n+2)!}\frac{d^{n+2}V(r_0)}{dr_0^{n+2}}\right]x^{n+2}.\quad (26)$$
Equation (9) thus becomes

\[
\left[ -\frac{1}{2} \frac{d^2}{dx^2} + \sum_{n=0}^{\infty} v^{(n)} \bar{l}^{-n/2} \right] \Psi_{n_r,l}(x) = \\
\left[ \frac{1}{l} \left( \frac{\beta(\beta+1)}{2} + \lambda_0^{(0)} \right) + \sum_{n=2}^{\infty} \lambda_{n_r}^{(n-1)} \bar{l}^{-n} \right] \Psi_{n_r,l}(x). \tag{27}
\]

When setting the nodeless, \( n_r = 0 \), wave functions as

\[ \Psi_{0,l}(x(r)) = \exp(U_{0,l}(x)), \tag{28} \]

equation (27) is readily transformed into the following Riccati equation:

\[
-\frac{1}{2} \left[ U''(x) + U'(x)U'(x) \right] + \sum_{n=0}^{\infty} v^{(n)}(x) \bar{l}^{-n/2} = \frac{1}{l} \left( \frac{\beta(\beta+1)}{2} + \lambda_0^{(0)} \right) \]
\[ + \sum_{n=2}^{\infty} \lambda_{0}^{(n-1)} \bar{l}^{-n}. \tag{29} \]

Hereinafter, we shall use \( U(x) \) instead of \( U_{0,l}(x) \) for simplicity, and the prime of \( U(x) \) denotes derivative with respect to \( x \). It is evident that this equation admits solution of the form

\[
U'(x) = \sum_{n=0}^{\infty} U^{(n)}(x) \bar{l}^{-n/2} + \sum_{n=0}^{\infty} G^{(n)}(x) \bar{l}^{-(n+1)/2}, \tag{30}
\]

where

\[
U^{(n)}(x) = \sum_{m=0}^{n+1} D_{m,n} x^{2m-1} ; \quad D_{0,n} = 0, \tag{31}
\]

\[
G^{(n)}(x) = \sum_{m=0}^{n+1} C_{m,n} x^{2m}. \tag{32}
\]
Substituting equations (30) - (32) into equation (29) implies

\[- \frac{1}{2} \sum_{n=0}^{\infty} \left[ U^{(n)} \bar{I}^{-n/2} + G^{(n)} \bar{I}^{-(n+1)/2} \right] \]

\[- \frac{1}{2} \sum_{n=0}^{\infty} \sum_{p=0}^{\infty} \left[ U^{(n)} U^{(p)} \bar{I}^{-(n+p)/2} + G^{(n)} G^{(p)} \bar{I}^{-(n+p+2)/2} + 2 U^{(n)} G^{(p)} \bar{I}^{-(n+p+1)/2} \right] \]

\[+ \sum_{n=0}^{\infty} v^{(n)} \bar{I}^{-n/2} = \frac{1}{\ell} \left( \frac{\beta(\beta + 1)}{2} + \lambda_0^{(0)} \right) + \sum_{n=2}^{\infty} \lambda_0^{(n-1)} \bar{I}^{-n}, \quad (33)\]

where primes of $U^{(n)}(x)$ and $G^{(n)}(x)$ denote derivatives with respect to $x$.

Equating the coefficients of the same powers of $\bar{I}$ and $x$, respectively, ( of course the other way around would work equally well) one obtains

\[- \frac{1}{2} U^{(0)}' - \frac{1}{2} U^{(0)} U^{(0)} + v^{(0)} = 0, \quad (34)\]

\[U^{(0)}'(x) = D_{1,0} \quad ; \quad D_{1,0} = -w, \quad (35)\]

and integration over $dx$ yields

\[U^{(0)}(x) = -wx. \quad (36)\]

Similarly,

\[- \frac{1}{2} \left( U^{(1)}' + G^{(0)}' \right) - U^{(0)} U^{(1)} - U^{(0)} G^{(0)} + v^{(1)} = 0, \quad (37)\]

\[U^{(1)}(x) = 0, \quad (38)\]

\[G^{(0)}(x) = C_{0,0} + C_{1,0} x^2, \quad (39)\]
\[ C_{1,0} = -\frac{B_1}{w}, \quad (40) \]

\[ C_{0,0} = \frac{1}{w}(C_{1,0} + 2\beta + 1), \quad (41) \]

\[ B_1 = -2 + \frac{r_0^3}{6Q} \frac{d^3 V(r_0)}{dr_0^3}, \quad (42) \]

\[
- \frac{1}{2} [U^{(2)'} + G^{(1)'}] - \frac{1}{2} \sum_{n=0}^{2} U^{(n)} U^{(2-n)} - \frac{1}{2} G^{(0)} G^{(0)} \\
- \sum_{n=0}^{1} U^{(n)} G^{(1-n)} + a^{(2)} = \frac{\beta(\beta + 1)}{2} + \lambda_0^{(0)}, \quad (43) 
\]

\[ U^{(2)}(x) = D_{1,2} x + D_{2,2} x^3, \quad (44) \]

\[ G^{(1)}(x) = 0, \quad (45) \]

\[ D_{2,2} = \frac{1}{w} \left( \frac{C_{2,0}^2}{2} - B_2 \right) \quad (46) \]

\[ D_{1,2} = \frac{1}{w} \left( \frac{3}{2} D_{2,2} + C_{0,0} C_{1,0} - \frac{3}{2} (2\beta + 1) \right), \quad (47) \]

\[ B_2 = \frac{5}{2} + \frac{r_0^6}{24Q} \frac{d^4 V(r_0)}{dr_0^4}. \quad (48) \]
\[ \lambda_0^{(0)} = -\frac{1}{2}(D_{1,2} + C_{0,0}^2). \]  

\[ (49) \]

\[ \cdots \text{and so on. Thus, one can calculate the energy eigenvalue and the eigenfunctions from the knowledge of } C_{m,n} \text{ and } D_{m,n} \text{ in a hierarchical manner. Nevertheless, the procedure just described is suitable for systematic calculations using software packages (such as MATHEMATICA, MAPLE, or REDUCE) to determine the energy eigenvalue and eigenfunction corrections up to any order of the pseudoperturbation series.} \]

Although the energy series, Eq.(8), could appear divergent, or, at best, asymptotic for small \( \bar{l} \), one can still calculate the eigenenergies to a very good accuracy by forming the sophisticated Pade’ approximation to the energy series. Our strategy is therefore clear.

### 3 Yukawa Potential

Let us begin with the Yukawa potential (1), where the screening parameter \( \alpha \) is given by the amended Z-dependent relation

\[ \alpha = 0.98Z^{1/3}(1 - 1/Z)^{2/3}. \]  

\[ (50) \]

Thus, Eq.(22) with \( n_r = 0 \) reads

\[ w = \sqrt{-\alpha^2 r_0^2 + \alpha r_0 + 1 \over \alpha r_0 + 1}, \]  

\[ (51) \]

and Eq.(20) in turn implies

\[ l + \frac{1}{2}(1 + w) = \sqrt{Zr_0 e^{-\alpha r_0}(\alpha r_0 + 1)}. \]  

\[ (52) \]

Evidently, one should appeal to numerical techniques to solve for \( r_0 \) since a closed form solution for Eq.(52) is hard to find, if it is feasible at all. Once \( r_0 \)
is determined the coefficients $C_{m,n}$ and $D_{m,n}$ are obtained in a sequel manner. Consequently, the eigenvalues and eigengfunctions are calculated in the same batch for each value of $Z$ and $\alpha$.

In tables 1 and 2, we list our K- and L-shell binding energies, measured in units of $2\text{Ry}=27.196 \text{ eV}$, for some values of $Z$ and compare with those of the hypervirial - Padé method (HPM) [18], and of the shifted large - N expansion technique (SLNT) [14]. In table 1, the results of Ecker - Weizel approximation (EWA) [16] are also displayed. The first ten terms of our energy series are calculated and the stability of the sequence of Padé approximants is considered.

Evidently, our results compare better with those of HPM than the results of SLNT. However, considering only the first four terms of our series, our results are found in exact agreement with those of SLNT. The accuracy of our results is enhanced by the Padé approximants which show stability all the way from $E[2,2]$ to $E[4,5]$. Such stability indicates that our results are exact, provided that some uncertainty lies in the last $j$ digits in parentheses.

On the other hand, one would pass to dimensionless quantities by scaling the Hamiltonian and reducing it to the form

$$H_y = -\frac{1}{2} \frac{d^2}{dy^2} + \frac{l(l+1)}{2y^2} - \frac{1}{y} e^{-\alpha'y},$$

where $y \in (0, \infty)$ and $\alpha'$ is a positive screening parameter. Then, to return back to dimensional quantities one has to make the following substitutions

$$y = Zr, \quad \alpha' = \frac{\alpha}{Z} = 0.98Z^{-2/3}(1 - \frac{1}{Z})^{2/3},$$

where $Z = 1, 2, 3, \cdots$. Therefore, $\alpha'$ can not be a random screening parameter. It is restricted by Eq.(54), which in effect implies that the lowest value of $\alpha'$ is zero when $Z = 1$ and immediately a maximum value 0.38891326 at $Z=2$. For $Z > 2$, $\alpha'$ decreases smoothly and converges to zero as $Z \to \infty$. To figure this out, one should simply sketch the relation of $\alpha'$ vs $Z$, given in Eq.(54). Hence, we proceed with our comparison, using only several eligible values for $\alpha'$, and list our results (tables 3 and 4) along with those of Varshni [11], via SLNT, Fernandez et al. [23], via a rational function approximation (RFA), and the
exact ones [24,25]. Our results, again, are in better agreement with the RFA and the exact ones than those of Varshni [11], via Papp's [12] or Imbo's [13] SLNT proposals.

Although we have used the atomic units through out, our energies in tables 1 and 2 are multiplied by 2Ry for the sake of comparison with the results from HPM [18], EWA [16], and SLNT [14].

4 Concluding remarks

In view of the results reported in tables 1-4, some remarks merit to be mentioned.

It is evident that working with the scaled Hamiltonian, Eq.(53), facilitates the calculations and enhances the accuracy of PSLET. As can be seen from our results, the convergence for the energy eigenvalues is extremely rapid when the scaled Hamiltonian is used. It should be obvious for the reader to see that all Z - values in tables 1-2 fall in the range of \( \alpha' \) in tables 3 and 4. Moreover, as \( \alpha' \) gets smaller the Yukawa potential becomes more Coulombic in nature, and when \( \alpha' = 0 \) at \( Z = 1 \) the Yukawa collapses into the exact Coulombic potential, for which PSLET gives exact spectrum from the leading term \( \bar{R}E^{(-2)} \) and higher - order corrections vanish identically.

The answer to the question as to why all methods reported by Varshni [11] give poor accuracies for \( \alpha' \geq 0.7 \), lies perhaps in the restriction provided by Eq.(54) that \( \alpha' < 0.4 \) (table 1 of ref.[11] bears this out). Moreover, the non-negligible deviations of SLNT results [19,20,26-30] from the exact values should be attributed, mainly, to the limited capability of SLNT to calculate the energy corrections beyond the fourth - order.

From the knowledge of \( C_{m,n} \) and \( D_{m,n} \) one can calculate, in the same batch, the wave functions to study electronic transitions and multiphoton emission occurring in atomic systems in the presence of intense laser fields, for example. Such studies already lie beyond the scope of our present methodical proposal.

To sum up, we have demonstrated that it is an easy task to implement PSLET without having to worry about the ranges of couplings and forms of perturbations in the potential involved. In contrast to the textbook Rayleigh - Schrödinger perturbation theory, an easy feasibility of computation of the eigenvalues and eigenfunctions, in one batch, has been demonstrated, and satisfactory
accuracies have been obtained. Moreover, a nice numerical trend of convergence
has been achieved. Nevertheless, another suitable criterion for choosing the
value of the shift $\beta$, reported in ref. [30], is also feasible. This reference should
be consulted for more details.
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Table 1: K-shell energies, with \( n_r = 0 \) and \( l = 0 \), in KeV for \( V(r) = -Ze^{-\alpha r}/r \).

Where \( E_{PSLET} \) represents PSLET results, \( E_{HPM} \) denotes the Hypervirial method [18], \( E_{EW_A} \) from [16], and \( E_{SLNT} \) from [14]. \( E[4, 5] \) is the \([4, 5]\) Padé approximant obtained by replacing the last \( j \) digits of \( E[4, 4] \) with the \( j \) digits in parentheses.

| \( Z \) | \(-E_{EW_A}\) | \(-E_{HPM}\) | \(-E_{SLNT}\) | \(-E_{PSLET}\) | \(-E[4, 4] \& (-E[4, 5])\) |
|-------|-------------|-------------|-------------|-------------|------------------|
| 3     | 0.05334     | 0.05415     | 0.05414     | 0.054135    | 0.05414708 (19)  |
| 6     | 0.274       | 0.27623     | 0.27623     | 0.276226    | 0.27622917 (22)  |
| 9     | 0.701       | 0.70461     | 0.70461     | 0.704612    | 0.70461288 (9)   |
| 14    | 1.897       | 1.90320     | 1.90320     | 1.903198    | 1.903198386 (6)  |
| 19    | 3.716       | 3.72545     | 3.72545     | 3.725447    | 3.725447269 (7)  |
| 24    | 6.171       | 6.18277     | 6.18277     | 6.182765    | 6.182765210 (07) |
| 29    | 9.268       | 9.28212     | 9.28213     | 9.282124    | 9.282124421 (18) |
| 34    | 13.012      | 13.02830    | 13.02830    | 13.028304   | 13.028303677 (4) |
| 39    | 17.407      | 17.42482    | 17.42482    | 17.424818   | 17.424817591 (88)|
| 44    | 22.454      | 22.47438    | 22.47438    | 22.474378   | 22.474378305 (3) |
| 49    | 28.157      | 28.17915    | 28.17915    | 28.179153   | 28.179153161 (0)|
| 54    | 34.517      | 34.54092    | 34.54092    | 34.540921   | 34.540920826 (5)|
| 59    | 41.535      | 41.56612    | 41.56117    | 41.56117189 | 41.561171872 (1) |
| 64    | 49.213      | 49.24118    | 49.24118    | 49.2411768  | 49.241176745 (4)|
| 69    | 57.553      | 57.58203    | 57.58203    | 57.5820335  | 57.58203349 (8)|
| 74    | 66.554      | 66.58470    | 66.58470    | 66.5847023  | 66.584702299 (9)|
| 79    | 76.217      | 76.25003    | 76.25003    | 76.2500313  | 76.250031268 (8)|
| 84    | 86.544      | 86.57878    | 86.57878    | 86.5787759  | 86.578775902 (1)|
Table 2: L-shell energies, with $n_r = 0$ and $l = 1$, in KeV for $V(r) = -Ze^{-\alpha r}/r$. Where $E_{PSLET}$ represents PSLET results, $E_{HPM}$ denotes the Hypervirial method [18], and $E_{SLNT}$ from [14]. $E[4,5]$ is the [4,5] Padé approximant obtained by replacing the last $j$ digits of $E[4,4]$ with the $j$ digits in parentheses.

| $Z$ | $-E_{HPM}$ | $-E_{SLNT}$ | $-E_{PSLET}$ | $-E[4,4]$ & $(-E[4,5])$ |
|-----|------------|-------------|--------------|-----------------|
| 9   | 0.00423    | 0.00437     | 0.0056       | 0.0041 (1)      |
| 14  | 0.08953    | 0.08945     | 0.08948      | 0.089523 (31)   |
| 19  | 0.28398    | 0.28394     | 0.283962     | 0.283977 (8)    |
| 24  | 0.59991    | 0.59989     | 0.599905     | 0.599912 (2)    |
| 29  | 1.04510    | 1.04508     | 0.045092     | 1.0450957 (8)   |
| 34  | 1.62485    | 1.62484     | 1.624851     | 1.6248535 (6)   |
| 39  | 2.34309    | 2.34308     | 2.343087     | 2.3430888 (9)   |
| 44  | 3.20280    | 3.20280     | 3.203800     | 3.2028012 (3)   |
| 49  | 4.20638    | 4.20637     | 4.2063780    | 4.20637855 (9)  |
| 54  | 5.35577    | 5.35577     | 5.3557723    | 5.35577266 (9)  |
| 59  | 6.65261    | 6.65261     | 6.6526133    | 6.65261354 (6)  |
| 64  | 8.09829    | 8.09828     | 8.0982857    | 8.09828593 (5)  |
| 69  | 9.69398    | 9.69398     | 9.6939829    | 9.69398303 (4)  |
| 74  | 11.44075   | 11.44074    | 11.4407452   | 11.44074536 (7) |
| 79  | 13.33949   | 13.33949    | 13.3394894   | 13.33948956 (7) |
| 84  | 15.39103   | 15.39103    | 15.3910302   | 15.39103029 (30)|

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Table 3: K-shell energies, with \( n_r = 0 \) and \( l = 0 \), in \( \hbar = m = e = 1 \) units for \( V(r) = -e^{-\alpha' r}/r \). Where \( E_{PSLET} \) represents PSLET results, \( E_{Papp} \) denotes SLNT, via Papps proposal [11], and \( E_{Imbo} \) SLNT, via Imbo’s proposal [11]. \( E[4,5] \) is the [4,5] Padé approximant obtained by replacing the last \( j \) digits of \( E[4,4] \) with the \( j \) digits in parentheses.

| \( \alpha' \) | \( -E_{Papp} \) | \( -E_{Imbo} \) | \( -E_{PSLET} \) | \( -E[4,4] \) & (\( -E[4,5] \)) | Exact [23-25] |
|--------------|-----------------|-----------------|-----------------|-------------------------------|----------------|
| 0.1          | 0.407058        | 0.407058        | 0.40705803      | 0.407058031 (1)               | 0.407058031    |
| 0.2          | 0.326808        | 0.326808        | 0.326808231     | 0.326808515 (9)               | 0.326808515    |
| 0.3          | 0.257634        | 0.257634        | 0.257628168     | 0.25763869 (8)                | 0.25763869     |
| 0.4          | 0.198346        | 0.198345        | 0.198260722     | 0.198377 (8)                  | 0.198377       |

Table 4: K-shell energies, with \( n_r = 0 \) and \( l = 0 \), in \( \hbar = m = e = 1 \) units for \( V(r) = -e^{-\alpha' r}/r \). Where \( E_{PSLET} \) represents PSLET results, \( E[4,5] \) is the [4,5] Padé approximant obtained by replacing the last \( j \) digits of \( E[4,4] \) with the \( j \) digits in parentheses.

| \( \alpha' \) | \( -E_{PSLET} \) | \( -E[4,4] \) & (\( -E[4,5] \)) |
|--------------|-----------------|-------------------------------|
| 0.01         | 0.4900745067    | 0.490074506746694 (4)         |
| 0.02         | 0.48029610598   | 0.48029610598378 (8)          |
| 0.03         | 0.4706620270266 | 0.4706620270246 (4)           |