

Convergent perturbation studies in screened coulomb potential systems: analytic evaluations up to third order for the Yukawa case

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This is the first of a series of papers on the perturbative treatment of screened coulomb potential systems in quantum mechanics. Its content is mainly devoted to the evaluation of first four terms in a convergent energy expansion of Yukawa potential. For this purpose, a weighted eigenvalue problem of Laplacian accompanied by spherical symmetry is employed to find the inverse of the Schrödinger operator for unperturbed case (which is assumed to be the Hamiltonian of Hydrogen-like systems). Some very encouraging numerical results are also given for illustrative purposes.

Key words: Perturbation theory – Screened coulomb potentials — Yukawa potential

1. Introduction

The screened coulomb potential has a great importance in quantum mechanics, especially in describing certain atomic phenomena involving electronic transitions. It has been investigated numerically and analytically by several procedures like the WKBJ method [1], quantum defect method [2], and several types of perturbation methods [3].

It is very convenient to separate the class of screened coulomb potentials into two categories, one of which only involves the cases where the difference between the screened coulomb potential and the limit potential when the screening parameter, say γ , goes to zero is bounded and the other of which includes the cases where the same difference is unbounded. The usefulness of this classification

lies in the fact that the boundedness of the perturbation operator strongly determines the convergence domain of perturbation series with respect to the perturbation parameter, say ε , for both eigenvalue and eigenfunction. Therefore, bounded perturbations will provide convergent perturbation series with a finite radius of convergence, however, the unbounded ones will result in perturbation series which are divergent at everywhere except at the origin of ε -complex plane [4].

There are several papers on the investigation of certain properties of the Schrödinger's equation's eigenvalue as a function of perturbation parameter ε for various structures of screened coulomb potential [5] in numerical [6], group theoretical [7-12], perturbative [13-17] treatments of the problem. However, we are not going to give more references about the subject and the reader is kindly invited to take a promenade in the world of abundant worthwhile works for gathering further information about the topic.

In this work, we revisit the convergent perturbation treatment for Yukawa potential realized by Smith [13] in 1964. There, only first order perturbative results are given. Here, we are going to proceed up to third order terms, the analytic expressions of which could be attained. Since, the second step of these series of works will involve the construction of an efficient, general purpose, numerical algorithm to evaluate the perturbative contributions up to any desired order we shall need exact values of, at least, first few contributions to check the performance of that algorithm via comparison of the algorithm's results with the analytical ones. Hence, obtaining such analytical results is a necessity rather than a mere satisfaction in mathematical elegance. On the other hand, the precision in the results evaluated by these formulae will reveal their utilizability in getting satisfactorily accurate values for the eigenvalues of Schrödinger's equation with Yukawa potential.

In the coming sections we shall present the evaluations of first four perturbative contributions to the energy for Yukawa system. The last section will, as usual, include the concluding remarks.

2. Formulation of the perturbation scheme and the evaluation of first-order contribution

Let us assume we have a quantum mechanical system in a central force field. This assumption of angle-independence in spherical coordinates, immediately makes it possible to write the radial equation for the eigenfunctions under l th order azimuthal symmetry via dimensionless coordinate and parameters as follows

$$-\frac{1}{2} \frac{d^2 \bar{\psi}}{dr^2} - \frac{1}{r} \frac{d\bar{\psi}}{dr} + \frac{l(l+1)}{2r^2} \bar{\psi} - \frac{V(\gamma r)}{r} \bar{\psi} = \bar{E} \bar{\psi}$$

$$r \in [0, \infty), \quad \bar{\psi} \in L_2 \quad (\text{the space of square integrable functions}) \quad (2.1)$$

where l , γ and \bar{E} denote, respectively azimuthal quantum number, screening parameter and energy eigenvalue. On the other hand, l th order azimuthal symmetry implies that the angle-dependence of the eigenfunctions can completely

be characterized by l th order spherical harmonics. Therefore, we have confined ourselves only to the angle-independent potential cases. Beyond this limitation, we shall also assume that $V(\gamma r)$ is a bounded function of its argument on the semi-interval $[0, \infty)$ and the normalization condition $V(0) = 1$ holds. Whenever $V(0)$ differs from unity one can immediately use a scaling transformation on radial variable and get the possibility of dealing with a new potential $\bar{V}(\bar{\gamma}r)$ such that $\bar{V}(0) = 1$ and $\bar{\gamma} = \gamma/V(0)$ hence, the last condition does not create any loss of generality. The limitation on the boundedness of $V(r)$ is due to the fact that the unbounded potential case can not be treated in the same way with the bounded potential case. Indeed, in those cases a different kind of expansion is needed to get accurate results by dealing with convergent perturbation series. In our future works, we are willing to deal with such a category of potential functions.

In the light of these discussions we can, now consider the Eq. (2.1) as a special case of the following, more general, equation

$$-\frac{1}{2} \frac{d^2\psi}{dr^2} - \frac{1}{r} \frac{d\psi}{dr} + \frac{l(l+1)}{2r^2} \psi - \frac{1}{r} \psi + \varepsilon \frac{1-V(\gamma r)}{r} \psi = E\psi$$

$$r \in [0, \infty), \quad \psi \in L_2. \tag{2.2}$$

Therefore, the equalities

$$\bar{\psi}(r) = \{\psi(r)\}_{\varepsilon=1} \tag{2.3}$$

$$\bar{E} = \{E\}_{\varepsilon=1} \tag{2.4}$$

are obvious. Henceforth, our task will be the determination of the serial expansions of $E(\varepsilon)$ and $\psi(r, \varepsilon)$ in nonnegative powers of ε . Since the perturbation potential

$$P(r) = \frac{1-V(\gamma r)}{r} \tag{2.5}$$

which measures the global deviation of the screened coulomb potential from the coulomb potential for hydrogen atom, is bounded; the perturbation theory of linear operators [4] dictates us that the resulting energy series will have, non-empty, at least finite, convergence regions in E -complex plane. Since the radius of this convergence circle depends on γ and it covers all E -plane when γ vanishes (hydrogen atom case, the perturbation series ends at the zeroth order term) we can expect that these series will converge as long as γ remains smaller than a non-zero value, say $\tilde{\gamma}$. If one can find that $\tilde{\gamma}$ reaches a critical value, γ_{cr} where the bound state under consideration cannot survive, then all eigen-energies of the system will be analytically determined. Even when this is not so, we shall be able to get the chance of analytic continuation from these limitedly convergent series to other values of γ via standard techniques.

Let us, now, assume the following expansions for $E(\varepsilon)$ and $\psi(r, \varepsilon)$ to be valid in a finite radius vicinity of the origin in ε -complex plane

$$E(\varepsilon) = \sum_{k=0}^{\infty} E_k \varepsilon^k, \quad \varepsilon \leq \rho_\varepsilon \tag{2.6}$$

$$\psi(r, \varepsilon) = \sum_{k=0}^{\infty} \psi_k(r) \varepsilon^k, \quad \varepsilon \leq \rho_\varepsilon, \quad r \in [0, \infty). \tag{2.7}$$

These immediately yield the following recursion in ψ_k 's (H_0 being unperturbed Hamiltonian of the system)

$$(H_0 - E_0 I)\psi_0 = 0 \tag{2.8}$$

$$(H_0 - E_0 I)\psi_k = \sum_{j=0}^{k-1} E_{k-j}\psi_j - P\psi_{k-1}, \quad k \geq 1 \tag{2.9}$$

where ψ_k 's are assumed to be in the Hilbert space of square integrable functions of r on the interval $[0, \infty)$ with a scalar product which has a weight r^2 . Eq. (2.8) produces the eigen states of hydrogen atom, hence one can start by choosing a specified eigenlevel of this system as follows

$$E_0 = -\frac{1}{2(n+l+1)^2}, \quad l = 0, 1, 2, \dots, n = 0, 1, 2, \dots \tag{2.10}$$

$$\psi_0(r) = \frac{2}{(n+l+1)^2} \left[\frac{n!}{(n+2l+1)} \right]^{1/2} \left\{ \frac{2r}{(n+l+1)} \right\}^l e^{-r/(n+l+1)} L_n^{2l+1} \left(\frac{2r}{n+l+1} \right) \tag{2.11}$$

where ψ_0 is normalized by unity and L_n^{2l+1} denotes the associated Laguerre Polynomial.

If we, now, take the scalar product of Eq. (2.9) by ψ_0 and consequently use the self-adjointness of H and the Eq. (2.8), we can conclude the following formula for E_k 's

$$\sum_{j=0}^{k-1} E_{k-j} \langle \psi_0, \psi_j \rangle - \langle \psi_0, P\psi_{k-1} \rangle = 0. \tag{2.12}$$

As is easily understood, the determination of E_1 necessitates only ψ_0 ,

$$E_1 = \frac{2}{(n+l+1)^2} \frac{n!}{(n+2l+1)!} \int_0^\infty x^{2l+1} e^{-x} \left[1 - V \left(\frac{n+l+1}{2} \gamma x \right) \right] \{L_n^{2l+1}(x)\}^2 dx \tag{2.13}$$

where the change of variable $x = 2r/(n+l+1)$ has been used.

Obviously, the evaluation of E_1 is just a matter of quadrature. Depending on the analytic structure of $P(x)$, one can perform it analytically or, at least, numerically. Since our aim is to get certain analytical formulae to be used for comparative purposes in our future works, we are going to specify V as follows

$$V(x) = e^{-x} \tag{2.14}$$

which is certainly Yukawa type of screening function. Therefore, after performing the integration in Eq (2.13) we find

$$E_1 = \frac{1}{(n+l+1)^2} \left[1 - \sigma_2 F_1 \left(\begin{matrix} -n, -n \\ -2n-2l-1 \end{matrix} \middle| 1 - \frac{4}{(n+l+1)^2 \gamma^2} \right) \right] \tag{2.15}$$

where ${}_2F_1$ denotes Gaussian hypergeometric function [18] and σ has the following expression

$$\sigma = \frac{(2n+2l+1)!}{n!(n+2l+1)!} \left[1 + \frac{(n+l+1)}{2} \gamma \right]^{-2n-2l-2} \frac{(n+l+1)^{2n}}{2^{2n}} \gamma^{2n}. \tag{2.16}$$

The result in Eq. (2.15) is a reproduction of Smith's [13] result. In his work he only proceeds up to first order and his purpose seemed to get a reasonably accurate, perturbative approach without cumbersome procedures. Indeed as is very well-known, higher order terms necessitate the evaluation of the inverse of the unperturbed Hamiltonian of the system, over the complementary subspace of the finite dimensional space spanned by the eigenvectors corresponding to a certain eigenvalue of H_0 . This task is generally difficult, tedious and discouraging when the continuous spectrum is involved in the spectrum of H_0 . However, the Hamiltonian of hydrogen atom makes it possible to deal with an operator, the spectrum of which is purely discrete [19]. Hence, we were able to analytically evaluate the second and third order contributions to energy. Although the evaluation of higher order terms seems to be, in principle, possible, the enormness of the effort needed to handle the intermediate steps without mistakes, has prevented us from continuing further in this direction. As a matter of fact, the scheme remains same in higher order evaluations, however the appearance of many dimensional integrations which are elementary in concept, rapidly increases the number of manipulations.

3. Second-order contribution to energy and first-order perturbative eigenfunction

Let us, now, consider the following inhomogeneous differential equation

$$(H_0 - E_0 I)f = \left\{ -\frac{1}{2} \frac{d^2}{dr^2} - \frac{1}{r} \frac{d}{dr} + \frac{l(l+1)}{2r^2} - \frac{1}{r} + \frac{1}{2(n+l+1)^2} \right\} f = \tilde{g} \tag{3.1}$$

where f and g belong to the space of square integrable functions over the weight r^2 . If we transform the variable r into x as follows

$$r = \frac{n+l+1}{2} x \tag{3.2}$$

we can conclude

$$[T - (n+l+1)I]f = g(x); g(x) = \frac{(n+l+1)}{2} x \tilde{g} \left(\frac{n+l+1}{2} x \right) \tag{3.3}$$

where

$$T = -x \frac{d^2}{dx^2} - 2 \frac{d}{dx} + \frac{l(l+1)}{x} + \frac{x}{4}. \tag{3.4}$$

The operator T has purely discrete spectrum and its eigenfunctions form a complete orthonormal basis set for $[0, \infty)$ with respect to the weight function x .

They are related to associated Laguerre polynomials as follows

$$\varphi_n = \left[\frac{n!}{(n+2l+1)!} \right]^{1/2} e^{-x/2} x^l L_n^{2l+1}(x) \quad (3.5)$$

$$T\varphi_n = (n+l+1)\varphi_n, \quad \int_0^\infty \varphi_m \varphi_n r dr = \delta_{mn} \quad (3.6)$$

If we now remember the orthogonality of the right-hand side of the Eq. (3.3) to the homogeneous solution of its left-hand side via weight r , we can write

$$f = \sum_{\substack{m=0 \\ m \neq n}}^\infty \frac{1}{m-n} \varphi_m(x) \int_0^\infty \varphi_m(\xi) \xi g(\xi) d\xi \quad (3.7)$$

where f is assumed to be orthogonal to φ_n .

By using integral representation of $1/(m-n)$ and summation theorem of Laguerre polynomials one can write

$$f(x) = x^l e^{-x/2} \int_0^1 \frac{dz}{z^{n-l}} \int_0^\infty \xi^{l+1} e^{\xi/2} [K(x, \xi, z) - S(x, \xi, z)] g(\xi) d\xi \quad (3.8)$$

where

$$S(x, \xi, z) = \sum_{j=0}^n \frac{j!}{(j+2l+1)!} z^j L_j^{2l+1}(x) L_j^{2l+1}(\xi) [1 + z^{2n-2j} - \delta_{jn}] \quad (3.9)$$

$$K(x, \xi, z) = \frac{(x\xi z)^{-l-1/2}}{1-z} e^{-z(x+\xi)/(1-z)} I_{2l+1} \left(2 \frac{\sqrt{x\xi z}}{1-z} \right). \quad (3.10)$$

In these formulae δ_{jk} stands for Kronecker delta and I denotes first kind modified Bessel function [20].

If we now identify g with $\{E_1 - (1 - \exp(-\gamma r))/r\}\psi_0$ we can express ψ_1 for $n=0$ in the following manner after certain intermediate steps

$$\begin{aligned} \psi_1(x) = & A_{n0} x^l e^{-x/2} \left\{ \lambda_1 (x-2l-2) \right. \\ & \left. + \int_0^1 \frac{dz}{z} [W^{2l+2}(0) - W(z)^{2l+2} e^{-[z/(1-z)]x(1-W(z))}] \right\} \end{aligned} \quad (3.11)$$

where

$$A_{n0} = \frac{2}{(n+l+1)^2} \left[\frac{n!}{(n+2l+1)!} \right]^{1/2}; \quad \lambda_1 = -\frac{(n+l+1)^2}{2} E_1 \quad (3.12)$$

and

$$W(z) = \left[1 + \frac{(n+l+1)\gamma(1-z)}{2} \right]^{-1}. \quad (3.13)$$

Although ψ_1 has a similar form for other n values, certain finite sums appear and n -times differentiation with respect to a dummy variable can be used to get rid of most of the sums and to be able to express ψ_1 in a more compact form. Indeed, if we specify $g(x)$ as $x^{l-1} e^{-(\frac{1}{2}+\sigma)x} P(x)$ where σ and $P(x)$ are given as a constant and a polynomial respectively, then we can conclude the following formula in the frame of this philosophy

$$\mathcal{L}g = x^l e^{-x/2} \left\{ P \left(\frac{d}{d\alpha} \right) \Omega \right\}_{\alpha=0} \tag{3.14}$$

where \mathcal{L} denotes the inverse of the operator $\{T - (n+l+1)I\}$ on the complement of the space spanned by φ_n and Ω is defined as below

$$\Omega = \int_0^1 \frac{dz}{z^{n+1}} \left\{ W^{2l+2}(\alpha, 0) \sum_{j=0}^n [\delta_{j,n} - z^j - z^{2n-j}] [1 - W(\alpha, 0)]^j L_j^{2l+1}(x) + \Omega_1 \right\} \tag{3.15}$$

$$\Omega_1 = W^{2l+2}(\alpha, z) e^{-[z/(1-z)]x[1-W(\alpha,z)]} \tag{3.16}$$

$$W(\alpha, z) = \frac{1}{1 + \sigma(1-z) - \alpha(1-z)}. \tag{3.17}$$

These formulae can be used in several steps of calculations to express ψ_k 's as certain multi dimensional integrals. However, we are not going to get into details of this matter anymore because it is out of the scope of our work.

Now, we can immediately write the following formula for E_2

$$E_2 = \frac{2}{(n+l+1)^2} \{ \langle \psi_0, \psi_1 \rangle + \lambda_1 \langle x\psi_0, \psi_1 \rangle - \langle e^{-\gamma(n+l+1)x/2} \psi_1, \psi_0 \rangle \} \tag{3.18}$$

where ket and bra notation imply the scalar products over the weight x .

After performing the necessary integrations to evaluate the scalar products appearing above, one can conclude the following formula for the second order perturbative energy

$$E_2 = -\frac{2}{(n+l+1)^2} \lambda_2 \tag{3.19}$$

$$\lambda_2 = \lambda_1^2 + \gamma \mathcal{A}^3 \lambda_1 - \frac{\mathcal{A}^4}{2} \{ \ln [\mathcal{A}(2-\mathcal{A})] - \mathcal{B} \} \tag{3.20}$$

$$\mathcal{A} = \frac{2}{2+\gamma}; \quad \mathcal{B} = \frac{\gamma^2}{4(1+\gamma)}$$

4. Third-order perturbative contributions to the energy

Third-order perturbative contribution to the energy, E_3 , can be expressed in terms of certain inner products including ψ_0, ψ_1 and certain elementary functions after

using the hermiticity of the operator \mathcal{L} and the definition of ψ_1 via \mathcal{L} in the definition of E_3 , as follows

$$E_3 = -\frac{2}{(n+l+1)^2} \lambda_3 \quad (4.1)$$

$$\lambda_3 = 2\lambda_2 \langle x\psi_0, \psi_1 \rangle + \lambda_1 \langle x\psi_1, \psi_1 \rangle + \langle \psi_1, \psi_1 \rangle - \langle e^{-[(n+l+1)\gamma x/2]} \psi_1, \psi_1 \rangle \quad (4.2)$$

We have not given the intermediate steps of this derivation for the sake of brevity. Due to the same reason we are not also going to give the details of the evaluations of the inner products appearing above. As a matter of fact, nothing is new in the calculations of these integrals and all steps are elementary however the manipulations are tedious. Hence we only give the results for these inner products when $n=0$, $l=0$ as follows

$$\langle x\psi_0, \psi_1 \rangle = -\lambda_1 - \frac{\gamma}{2} \mathcal{A}^3 \quad (4.3)$$

$$\langle x\psi_1, \psi_1 \rangle = 4\lambda_1^2 - 6\mathcal{A}^2 \lambda_1^2 + \gamma \mathcal{A}^3 \lambda_1 + \mathcal{A}^5 \mathcal{B} + \mathcal{A}^4 \mathcal{S}_1 - 2\mathcal{A}^5 \ln[\mathcal{A}(2-\mathcal{A})] \quad (4.4)$$

$$\mathcal{S}_1 = \sum_{k=1}^{\infty} \frac{(1-\mathcal{A})^{2k}}{k^2} \quad (4.5)$$

$$\langle \psi_1, \psi_1 \rangle = \lambda_2 + \frac{\mathcal{A}^4}{2} (\mathcal{S}_1 - \mathcal{B}) \quad (4.6)$$

$$\begin{aligned} \langle e^{-\gamma x/2} \psi_1, \psi_1 \rangle &= \lambda_1^2 \mathcal{A}^2 (3\mathcal{A}^2 - 4\mathcal{A} + 2) + \lambda_1 \frac{\mathcal{A}^4}{1-\mathcal{A}} \left[\frac{1}{(2-\mathcal{A})^2} - \mathcal{A}^2 \right] \\ &- \lambda_1 \mathcal{A}^5 \gamma [\ln \mathcal{A}(2-\mathcal{A}) - \mathcal{B}] - \mathcal{A}^5 \ln(1-C^2) \left[\mathcal{B} + \frac{1}{2(2-\mathcal{A})} \right] \\ &- \frac{\mathcal{A}^6}{4} \ln^2(1-C^2) + \frac{\mathcal{A}^6}{2} [\ln^2 \mathcal{A}(2-\mathcal{A}) - 2\mathcal{B} \ln \mathcal{A}(2-\mathcal{A}) - \mathcal{S}_2] \end{aligned} \quad (4.7)$$

$$\mathcal{S}_2 = \sum_{k=1}^{\infty} \frac{(-1)^k}{k^2} \frac{(1-\mathcal{A})^{2k}}{(3-2\mathcal{A})^k} \quad (4.8)$$

$$C = (1-\mathcal{A})/(2-\mathcal{A}) \quad (4.9)$$

where \mathcal{S}_1 and \mathcal{S}_2 are very closely related to Lerch's transcendental [21] or incomplete zeta function, in other words they are well-known functions.

5. Results and concluding remarks

In the previous sections we have given the necessary and sufficient information to find the analytic expressions for first four contributions to the perturbation series of energy E_0, E_1, E_2, E_3 . Here, we present some calculations based on these kinds of formulae in Tables 1-4. In the first table the comparison of the consecutive cumulative values of first four contributions ($E_0, E_0 + E_1, \dots$) are given for $1s$ -state ($n=0, l=0$) at certain different γ -values. The results in

Table 1. The comparison of cumulative perturbational energy values for 1s-state

Screening parameter	Our results				C.S. Lai [15]	Rogers et al. [6]	Vrscay ^a [17]
	γ	E_0	$E_0 + E_1$	$E_0 + E_1 + E_2$	$E_0 + E_1 + E_2 + E_3$	1980	1970
0.05	-0.5	-0.451814	-0.45181642	-0.4518164284	—	—	—
0.10	-0.5	-0.40703	-0.4070575	-0.40705802	-0.40706	-0.4071	-0.4070580306
0.20	-0.5	-0.3264	-0.32679	-0.3268067	-0.32681	-0.3268	-0.3268085113
0.25	-0.5	-0.2901	-0.2909	-0.290912	-0.29092	-0.2909	—
0.50	-0.5	-0.140	-0.1464	-0.14761	-0.14812	-0.1481	-0.1481170218
1.00	-0.5	0.06	0.017	0.005	-0.01027	-0.01029	-0.0102857899

^a Only ten digits are quoted here

Table 2. The comparison of cumulative perturbational energy values for 2s-state

Screening parameter	Our results				C.S. Lai [15]	Rogers et al. [6]	Vrscay [17]
	γ	E_0	$E_0 + E_1$	$E_0 + E_1 + E_2$	$E_0 + E_1 + E_2 + E_3$	1980	1970
0.05	-0.125	-0.0817	-0.08177	-0.0817710	-0.08177	-0.08177	-0.0817711957
0.10	-0.125	-0.049	-0.0498	-0.04991	-0.04993	-0.04993	-0.0499282713
0.20	-0.125	-0.005	-0.0100	-0.01118	-0.01211	-0.01211	-0.0121078651
0.25	-0.125	0.009	0.002	-0.0007	-0.00339	-0.00339	-0.0033959062
0.30	-0.125	0.02	0.01	0.006	-0.00005	—	-0.0000000379

Table 3. The comparison of cumulative perturbational energy values for 2p-state

Screening parameter	Our results				C.S. Lai [15]	Rogers et al. [6]	Vrscay [17]
	γ	E_0	$E_0 + E_1$	$E_0 + E_1 + E_2$	$E_0 + E_1 + E_2 + E_3$	1980	1970
0.05	-0.125	-0.0807	-0.08074	-0.0807402	-0.08074	-0.08074	-0.0807403870
0.10	-0.125	-0.0458	-0.04642	-0.046511	-0.04653	-0.04654	-0.0465343904
0.20	-0.125	0.04	-0.001	-0.0024	-0.00404	-0.00410	-0.0041016465

literature are also included to illustrate the convergence rate of the present perturbative scheme. Second and third tables include the same type of comparison for $2s(n=2, l=0)$ and $2p(n=0, l=1)$ states. The content of the last table, however, covers the comparison of the discrepancies between the sum $E_0 + E_1 + E_2 + E_3$ and the results obtained by Lai for several n, l and γ values.

As can be easily concluded, one can obtain quite high accuracy for sufficiently small γ values. In other words, the convergence rate of the perturbation series

Table 4. The discrepancies of third order cumulative perturbational energy values for various states

State	Screening parameters γ	Our results $E_0 + E_1 + E_2 + E_3$	C.S. Lai [15] 1980
3s	0.025	-0.0343294	-0.03433
3s	0.050	-0.019338	-0.01935
4s	0.025	-0.0124997	-0.01250
3p	0.025	-0.0340788	-0.03408
4p	0.025	-0.0122906	-0.01229
3d	0.025	-0.0335729	-0.03357
4d	0.025	-0.011866	-0.01187
4f	0.025	-0.011214	-0.01122

decreases as γ increases. On the other hand, convergence rate reduction seems not to depend on n and l . These observations imply that the perturbation series presented here, have limited convergence radius ($\tilde{\gamma}$) which depends on γ , n and l . If one can prove that $\tilde{\gamma}$ is equal to or greater than γ_{cr} which is the largest screening parameter value where the corresponding bound state can survive then we can use the present approach without any trouble. Toward this end an intense study is continuing.

Finally, it should be noticed that by using a bounded perturbation term in Schrödinger's equation, the presented convergent perturbation series have been constructed. The general tendency in this kind of perturbational problem is, however, to employ the screening constant, γ , as a perturbation parameter. The resulting series are divergent due to the existence of unbounded terms in the expansion of potential function with respect to the powers of γ , but certain acceleration techniques for instance Padé or Padé-Borel resummations yield quite accurate numerical results [17].

On the other hand, our approach may have some connections with the methods of deriving closed quadratures. However, as is cited in [22], there are serious problems extending the method to many dimensional cases. Since the evaluations appearing in certain perturbative steps are in quite general character and the increase of dimension alters nothing except the dimension of various integrals, our method becomes preferable. If the dimension of the integrals increases, the analytic evaluations will be too complicated. But, these type of integrals can be treated by truncated matrix representation of several operators appearing in their kernels and sufficiently accurate numerical results may be obtained. Indeed, a numerical algorithm to calculate any desired order contribution to the energy for any desired bounded screened coulomb potential is being developed. Work on, this subject is close to completion.

References

1. Foldy LL (1958) Phys Rev 111:1093
2. Seaton MJ (1958) Mon Not R Astron Soc 118:504

3. Pratt RH, Tseng HK (1972) Phys Rev A5:1063
4. Kato T (1966) Perturbation theory for linear operators. Springer, Berlin Heidelberg New York
5. Mehta CH, Patil SH (1978) Phys Rev A17:34
6. Rogers FJ, Graboske HC, Harwood DJ (1970) Phys Rev A1:1577
7. Gazeau JP, Maquet A (1979) Phys Rev A20:727
8. Barut AO (1972) Dynamical groups and generalized symmetries in quantum theory. University of Canterbury Publications, Christchurch, New Zealand
9. Bednar M (1973) Ann Phys 75:305
10. Cizek J, Vrscay ER (1982) Int J Quantum Chem 21:27
11. Adams BG, Cizek J, Paldus J (1982) Int J Quantum Chem 21:153
12. Rotenberg M (1970) Adv Atom Mol Phys, vol 6. Academic Press, New York
13. Smith CR (1964) Phys Rev 134:A1235
14. Grant M, Lai CS (1979) Phys Rev A20:718
15. Lai CS (1981) Phys Rev 23:455
16. McEnnan J, Kissel L, Pratt RH (1976) Phys Rev A13:532
17. Vrscay ER (1986) Phys Rev A33:1433
18. Luke YL (1969) The special functions and their approximation, vol I. Academic Press, New York
19. Demiralp M (1983) J Math Phys 24:101
20. Abramowitz M, Stegun IA (1970) Handbook of mathematical functions with formulas, graphs, and mathematical tables. Dover Publication, New York
21. Magnus W, Oberhettinger F, Soni RP (1966) Formulas and theorems for the special functions of mathematical physics. Springer, Berlin Heidelberg New York
22. Privman V (1981) Phys Rev: A24:2362