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An auto-coherent variational scheme for Yukawa potential

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The variational principle is used to obtain solutions to Schrödinger's equation for a particle in the Yukawa potential. A Laguerre basis set extended by an extra function is employed in the calculations. A special parameter used in the extra function and its relation with the systems energy results in utilizing an auto-coherent scheme. Considerable improvement seems to be achieved especially in the critical region where the screening parameter approaches its threshold value.

1. Introduction

The Schrödinger equation for a particle bound in a screened Coulomb potential is given by

$$\left\{-\frac{1}{2}\nabla^2 - \frac{1}{r}V(\gamma, r)\right\}\psi = E\psi; \quad \psi \epsilon \mathcal{H}, \tag{1.1}$$

where $\mathcal{H}$ is the Hilbert space of the problem and $V(\gamma, r)$ is a screening function with a screening parameter γ. If the function is chosen so that it is dependent solely on the radial variable r, one arrives at the radial form of (1.1)

$$\left\{-\frac{1}{2}\frac{d^2}{dr^2} - \frac{1}{r}\frac{d}{dr} + \frac{l(l+1)}{2r^2} - \frac{1}{r}V(\gamma, r)\right\}\psi = E\psi. \tag{1.2}$$

The wave functions of (1.1) and (1.2) are related to each other by spherical harmonics and l is the azimuthal quantum number. The boundary conditions of (1.2) are the continuity, the regularity and the vanishing behavior of ψ as r approaches infinity. The equation given by (1.2) is equivalent to solving the eigenvalue problem

of a self-adjoint operator under the weight r^2. This problem will yield a countably infinite or a finite number of discrete eigenvalues. The eigenfunctions corresponding to these eigenvalues belong to the set of functions that are continuous everywhere on the domain of $r\epsilon[0,\infty)$ and are square-integrable in the interval $[0,\infty)$ under the weight r^2. On the other hand, the decaying behavior of the potential as $r\to\infty$ implies that E will have both continuous and discrete spectra. The eigenfunctions corresponding to the continuous spectrum show a fluctuating slow decay behavior as r approaches infinity. In other words they belong to the class of functions which are square-integrable to the distribution (i.e. the delta function).

The screening function is often chosen so that it is finite in the domain $r\in[0,\infty)$ and that as $r\to\infty$ it approaches a constant value. Generally speaking, V is chosen so as to yield a constant for $\gamma=0$. For example, in the case of the Yukawa potential [1],

$$V(\gamma,r)=\mathrm{e}^{-\gamma r} \tag{1.3}$$

the afore-mentioned limits will be as follows:

$$V(0,r)=1\,, \tag{1.4}$$

$$V(\gamma,\infty)=0\,. \tag{1.5}$$

In other words for $\gamma=0$, (1.2) will become the electronic Schrödinger equation for a hydrogen-like atom, the solution of which can be found in any relevant textbook. On the other hand if γ is positive (i.e. not zero) the solutions of (1.2) are by no means trivial. The particle in question is under the effect of the central force field created by other charged particles. The strength of this field is determined by the size of the screening parameter. The larger the value of γ the heavier the screening and the less similar the system is to the hydrogen atom.

When γ is altered from zero in very small increments, the hydrogenic spectrum starts to move towards the continuum. And the number of the discrete states whose corresponding energies are negative immediately drops to a finite number. This is due to the fact that an infinite number of discrete states are pushed into the continuous spectrum. Obviously an accompanying structural change in the eigenfunctions of the problem occurs. The γ values which create these changes are named "critical" or "threshold" values of the screening parameter and to every state there corresponds a specific such value.

The Schrödinger equation with its screening function chosen as that proposed by Yukawa is perhaps the most commonly used test model to investigate the spectral structure of the screening phenomena.

The Yukawa potential arises naturally as the position-space version of the solution of the Klein–Gordon equation for a static meson field [1,2]. It was the deuteron problem which inspired the first solutions to the corresponding eigenvalue equation. It is also commonly known in plasma physics with the name "Debye–Hückel" potential and represents the effect of the plasma sea on localized two-particle inter-

actions [3–7]. In the calculation of the energy levels of impurity centers in doped semi-conductors the Debye–Hückel potential also approximates the Thomas–Fermi potential [8,9]. The Yukawa potential, together with Hulten's [10] and the exponential, plays an important role as a good test case in potential scattering studies, too. In quantum chemistry the effect of the core electrons on the valence electrons can be modelled via a linear combination of Yukawa or like potentials. To summarize an abundant literature on screened Coulomb potentials, it can be stated that the Yukawa potential is perhaps the most abundantly used formalism to represent a static radial shielding of a Coulomb potential.

Various approaches have been suggested to solving the eigenvalue problem associated with the corresponding Schrödinger equation having Yukawa or similar potentials. An abundant number of these use the variational [4,5,8–14] and the perturbational [4–6,11,12,15–21] techniques. Group theoretical approaches have also been employed by quite a few authors [22–24]. Direct numerical integration of the relevant Schrödinger equation has been reasonably successful, too [25–30]. Regge trajectories were determined via this means or by using continued-fraction expansions. Recently developed algebraic techniques were only partly successfull in determining ground state eigenvalues [31,32]. One of the most accurate energy values was given by Vrscay [19] in his recent attempt to analyze the behavior of the Padé approximants used by Lai [17]. The energy values were given to twenty decimal points for a sizeable screening domain for the 1s and the 2s states with obvious loss of accuracy for large screening parameters of the 2p state. A multiple-precision floating-point arithmetic package was used to get these results and moreover the Stieltjes behavior of Padé series assumed by Lai has proven to be false; leaving open the questions as to when and where the Padé approximant sequences of Lai will converge. An alternative route to solving the Schrödinger equation with Yukawa potential has been to approximate these potentials, as best as one can, with other potentials that can either be analytically solved or are relatively easier to tackle. One such work of considerable interest is that of Dutt et al. [33]. The Yukawa potential, together with the angularly dependent term is approximated by an Eckar [34] type potential, extending the Eckar–Weizel [3] approximation to the non-zero angular momentum states. The closeness of their energies to Yukawa energies are certainly encouraging. Lam and Varshni [11,12] followed by Dunlap and Armstrong [35] use the Hulten potential to approximate the $l = 0$ states of the Yukawa potential. Their results seems to fail quite badly as the screening parameter approaches its critical value.

The present authors have been involved in research on Yukawa potential for some time. Besides application of algebraic techniques [31,32] to Yukawa potential; perturbative [20,21] and variational [36] methods were also employed. A hydrogen-like operator was perturbed by a bounded operator in ref. [20,21]. An expansion in terms of a Laguerre basis set was employed to obtain the inverse of the operator. The results obtained are accurate to thirty decimal points for relatively low γ values. Chose to the critical regions, however, there is a quick loss of accu-

racy. Nevertheless, this partial success has led to utilizing Laguerre polynomials as a basis set in a variational treatment. These variational results were of similar nature and even slightly better in the critical region. A basis set comparison with the Eckart set showed that these were most promising in the critical region.

Eigenfunctions corresponding to eigenvalues away from the threshold are likely to be characterized quite well by a Laguerre set since these eigenfunctions will be most effective in the region where $r = 0$ and since the Laguerre polynomials are made up of powers of r. Therefore this basis set will represent the behavior of the exact solution around $r = 0$ rather well but will gradually loose its power as r increases. Approaching the threshold value implies that the function to be characterized is dominant in the region away from $r = 0$ where the Laguerre set has lost its effectiveness. This naturally implies that to get reasonable eigenfunctions and eigenvalues corresponding to screening parameters close to the threshold value, the basis set to be utilized must be extended by function(s) that can mimic the decaying behavior of the exact wave function.

In fact one of the present authors has used a rather similar approach to solve an eigenvalue problem which gives the critical values of the screening parameter [37]. There eq. (1.2) of the present paper was converted to a weighted eigenvalue problem after setting E equal to zero and utilizing a scaling transformation which leaves the screening function independent of the screening parameter. This created a proportionality constant for the potential term, the value of which depended on the critical value under investigation. Therefore the potential term became a weight-function for the eigenvalue problem of the critical values. The numerical solution of this eigenvalue problem could only be effectively realized by using an extended function in addition to Laguerre polynomials.

The formulation of the scheme will be covered in section 2, followed in section 3 by analytic evaluation of the matrix elements employed. Sections 4 and 5 will consecutively include results and concluding remarks.

2. Formulation of the scheme

The variational treatment of the eigenvalue problem given by (1.2) using a trial functions, ψ_T as a linear combination of a set of Φ_i's such that

$$\psi_T = \sum_{i=0}^{m} c_i \Phi_i \tag{2.1}$$

will lead to the matrix eigenvalue problem

$$\mathbf{Ac} = E\mathbf{Bc}\,, \tag{2.2}$$

where $\mathbf{A}$ is the Hamiltonian matrix given by

$$A_{ij} = \int_0^\infty \Phi_i H \Phi_j r^2 \, dr \tag{2.3}$$

in terms of the Hamiltonian operator H, defined as

$$H \equiv -\frac{1}{2}\frac{d^2}{dr^2} - \frac{1}{r}\frac{d}{dr} + \frac{l(l+1)}{2r^2} - \frac{1}{r}V(\gamma, r) \tag{2.4}$$

and **B** is the weight matrix (known also as the overlap matrix) given by

$$B_{ij} = \int_0^\infty \Phi_i \Phi_j r^2 \, dr . \tag{2.5}$$

The vector **c** contains the expansion coefficients c_i. If ϕ_i's are chosen so that they are orthonormal under the weight r^2, matrix **B** will turn into an $(m+1) \times (m+1)$ unit matrix and the weighted eigenvalue problem will turn into the unweighted eigenvalue problem

$$\mathbf{Ac} = E\mathbf{c} \tag{2.6}$$

the advantages of which will be quite apparent within the context of the autocoherent scheme to be discussed. The considerable success of the Laguerre basis set of ref. [36] suggests using basically the same set for the variational calculations in hand. Namely, Φ_i's will be chosen as

$$\Phi_i = \mathcal{N}_i y^l e^{-\frac{y}{2}} L_i^{2l+2}(y) , \tag{2.7}$$

where $y = 2\zeta r$ and ζ is a convergence acceleration parameter [36]. The set will be orthonormal under the weight r^2 and the normalization factor is

$$\mathcal{N}_i = (2\zeta)^{\frac{3}{2}} \left[\frac{i!}{(i+2l+2)!} \right]^{\frac{1}{2}} . \tag{2.8}$$

As discussed in detail in the previous section however, this basis set is not appropriate for γ values close the continuum threshold and it is necessary to reflect also the $r = \infty$ behavior of the exact solution of the equation (1.2) to the trial function to be utilized. To this end a perturbational approach can be developed. Defining a new parameter ν, through the relation $E = -\nu^2/2$, eq. (1.2) can be rewritten in the form

$$\left\{ -\frac{1}{2}\frac{d^2}{dr^2} - \frac{1}{r}\frac{d}{dr} + \frac{l(l+1)}{2r^2} + \frac{\nu^2}{2} \right\} \psi = \frac{\sigma}{r} V(\gamma, r) \psi , \tag{2.9}$$

where σ is later to be replaced by one. Choosing θ_k's independent of σ, the following expansion can be suggested:

$$\psi = \sum_{k=0}^{\infty} \sigma^k \theta_k . \tag{2.10}$$

In doing so, it is kept in mind that for $r \to \infty$ the potential will decay and the system will begin to characterize a free particle. Hence the relation

$$\left\{-\frac{1}{2}\frac{\mathrm{d}^2}{\mathrm{d}r^2}-\frac{1}{r}\frac{\mathrm{d}}{\mathrm{d}r}+\frac{l(l+1)}{2r^2}+\frac{\nu^2}{2}\right\}\theta_k=\frac{1}{r}V(\gamma,r)\theta_{k-1},\quad k\geqslant 0,\quad \theta_{-1}=0\,, \tag{2.11}$$

is achieved and for $k=0$ a solution can be constructed in terms of the modified spherical Bessel functions. There will be two linearly independent solutions and the one with the decaying behavior for $r\to\infty$ should be kept and the other discarded. This solution can be symbolically written as $Y_0\theta_0$. The following equation will be achieved for θ_1:

$$\theta_1 = Y_1\theta_0 + Y_0\int_r^\infty G(r,x)\frac{V(\gamma,x)}{x}\theta_0(x)\,\mathrm{d}x\,. \tag{2.12}$$

In this equation, G represents the Green function arising from the inversion of the operator acting on θ_k in eq. (2.11). It gives the decaying behavior to perturbative contributions. In general and specifically for $l\neq 0$ values, G has a rather complicated structure but does, however, contain a finite number of elementary functions. If the following definition is made:

$$\mathcal{K}\theta_0 \equiv \int_r^\infty G(r,x)\frac{V(\gamma,x)}{x}\theta_0(x)\,\mathrm{d}x\,, \tag{2.13}$$

then the relation

$$\theta_k = \sum_{i=0}^{k} Y_i\mathcal{K}^{k-i}\theta_0 \tag{2.14}$$

will be obtained. As $r\to 0$, $\mathcal{K}$ will have a polar singularity (at times a logarithmic one). The same is true for θ_0. Since the linear combination of θ_k's can be used as a trial function, a function constructed as

$$\Phi = \sum_{k=0}^{M} Y_k\mathcal{K}^k\theta_0 \tag{2.15}$$

can be used as the trial function. Here, the coefficients Y_k should be chosen so that the function Φ will not have a singularity at $r=0$. The perturbational approach developed is however, highly costly due to the nested integrals it involves. As a first approximation M is taken as one and the one-dimensional integral obtained is approximated by a properly chosen function so as to ensure the regularity condition at the origin.

In the Yukawa case an exponential type integral is encountered and replaced with its asymptotic form. An exponential parameter is used to characterize the errors arising from the asymptotic approximation of the integral and to keep the numerical convergence under control.

Due to the costly nature of the integration procedure, the nested integral structure is avoided by utilizing an extended Laguerre basis set which is composed of the

m members of the Laguerre basis set augmented by a function chosen via the above discussion. The perturbational analysis suggests that the extra function contains a combination of Modified Bessel Functions [38] so as to yield a decaying behavior as r approaches infinity. The Bessels will have (νr) as arguments so that the factor $e^{-\nu r}$ appears in the structure of the extra function, where ν is related to the eigenfunctions as stated before. This linear combination can be conveniently rewritten in the form

$$e^{-\nu r} \sum_{p=0}^{l} \frac{(l+p)!}{p!(l-p)!} (2\nu r)^{-(p+1)} . \tag{2.16}$$

Although this will have the correct behavior as $r \to \infty$, it will not be regular at $r = 0$. Therefore, to get an extra function with the correct behavior not only at infinity but also at zero, (2.16) has to be multiplied by a factor which will tend to one as $r \to \infty$ and will have an overall effect of r^l on the extra function at $r = 0$. This factor should preferably contain the potential function $V(\gamma, r)$ and be chosen such that the relevant integrals are reasonably easy to tackle. The function defined as

$$\Phi = \mathcal{D} e^{-\nu r} \sum_{p=0}^{l} \frac{(l+p)}{p!(l-p)!} (2\nu r)^{-(p+1)} [1 - e^{-\mu r}]^{2l+1} , \tag{2.17}$$

where $\mathcal{D}$ is a normalization constant and μ a parameter related to γ fulfills these requirements and was utilized as an augmentation to the Laguerre basis set of (2.7) for the Yukawa case.

To ensure an unweighted matrix eigenvalue problem rather than a weighted one, the extra function is to be chosen by Gram–Schmidt orthonormalization of Φ to all the m Laguerre bases. That is,

$$\Phi_m = \mathcal{N}_m \left[\Phi - \sum_{i=0}^{m-1} \beta_i \Phi_i \right] , \tag{2.18}$$

where

$$\beta_i = \int_0^\infty \Phi_i r^2 \, dr \tag{2.19}$$

and $\mathcal{N}_m$ is the relevant normalization factor given by

$$\mathcal{N}_m = \left[1 - \sum_{i=0}^{m-1} \beta_i^2 \right]^{-1/2} . \tag{2.20}$$

Hence the $r \to \infty$ behavior of the radial Schrödinger equation with the Yukawa potential suggests that the extra function Φ has a multiplicative factor $e^{-\nu r}$. Unlike the parameter α, ν is not a convergence accelerating parameter but has to be related to energy by the formula

$$E = -\tfrac{1}{2}\nu^2 . \tag{2.21}$$

Note that ν is always positive for discrete states and the corresponding energy is always negative. To proceed with a variational scheme by using augmented basis set composed of m Laguerre basis functions plus the extra function, one has to start with assigning a specific value to the parameter ν. Since the $\gamma = 0$ case corresponds to the hydrogenic atom and γ_{cr} to an energy value of zero, ν has to lie in $(0, 1]$ for the ground state. Given a ν value, the variational matrix **A** can be constructed, diagonalized and an E value can be obtained. This E can now be used to reconstruct a new starting ν value and so on. This procedure is to be repeated until consecutive E values are consistent to within a previously specified ϵ value. This is obviously an "auto-coherent scheme". We preferred the word "auto-coherent" to prevent any misinterpretation and confusion instead of the word "self-consistent" which is employed traditionally to imply certain group of methods. Since the augmented basis set spans only a subspace of the Hilbert space under consideration, m must be incremented say by Δm, and this process must be repeated until auto-coherent E values stabilize to within a desired accuracy. Evidently one can talk about the auto-coherency of a specific eigenstate and the interval for ν will be narrowed as the higher eigenstates are seeked.

3. Evaluation of the matrix elements

The matrix **A** and **B** of (2.2) have to be evaluated in three parts. First, the matrix elements corresponding to two bases, both of which are Laguerre type, will be evaluated (i.e. $A_{i,j}$ and $B_{i,j}$ where $i, j = 0, \ldots, m-1$), followed by the case where only one of the two bases is Laguerre type and the other is the extended basis (i.e. $A_{i,m}$ and $B_{i,m}$ or the symmetric elements $A_{m,i}$ and $B_{m,i}$ where $i = 0, \ldots, m-1$). Finally the diagonal elements $A_{m,m}$ and $B_{m,m}$ will be given (i.e. the case that corresponds to Φ and Φ).

To evaluate the first two cases, it is convenient to start by looking at the effect of the Hamiltonian operator H of eq. (2.4) on a function ξ_i, defined as

$$\xi_i = \mathcal{A}_i y^l \mathrm{e}^{-y/2} L_i^{\alpha}(y) , \tag{3.1}$$

where $\mathcal{A}_i$ is a normalization constant, α is a positive integer related to the azimuthal quantum number l and y is as defined in eq. (2.7). The result will be

$$H\xi_i = \zeta^2 \left\{ -\frac{1}{2}\xi_i + \frac{2(i+l+1)}{y}\xi_i + \frac{[\alpha-(2l+1)]}{y^2}\left(i\xi_i + [i+\alpha]\left[\frac{\mathcal{A}_i}{\mathcal{A}_{i-1}}\right]\xi_{i-1}\right)\right\} - \frac{V(\gamma, r)}{r}\xi_i . \tag{3.2}$$

The choice of the basis set given by (2.7) corresponds to an α value of $(2l+2)$. This will require that in the evaluation of the **A** matrix of (2.3) all the terms of (3.2)

will survive leading to rather tedious integrations. An alternative route is to employ a basis set defined as

$$\bar{\Phi} = \bar{\mathcal{N}}_i y^l \mathrm{e}^{-y/2} L_i^{2l+1}(y)\,, \tag{3.3}$$

which will be orthonormal under the weight r so that the normalization factor is

$$\bar{\mathcal{N}}_i = (2\zeta)\left[\frac{i!}{(i+2l+1)!}\right]^{1/2}. \tag{3.4}$$

This means that an α value of $(2l+1)$ is used in (3.1) which causes the third term in (3.2) to drop out. This results in much easier matrix evaluations.

The scheme followed will be to construct matrices $\bar{\mathbf{A}}$ and $\bar{\mathbf{B}}$ in terms of the $\bar{\Phi}_i$'s of (3.3) corresponding to the matrices **A** and **B** of (2.3) and (2.4) which were defined in terms of Φ_i's of (2.7) and then using the linear transformation

$$\Phi_i = \mathcal{N}_i \sum_{k=0}^{i} (\bar{\mathcal{N}}_k)^{-1} \bar{\Phi}_k \tag{3.5}$$

obtain the final **A** matrix.

$\bar{\mathbf{B}}$ turns out to be a tridiagonal matrix with relevant elements given as follows:

$$\bar{B}_{i,i} = \frac{(i+l+1)}{\zeta}\,,$$

$$\bar{B}_{i,i+1} = -(2\zeta)^{-1}[(i+1)(i+2l+2)]^{1/2}\,,$$

$$\bar{B}_{i+1,i} = \bar{B}_{i,i+1}\,. \tag{3.6}$$

The matrix $\bar{\mathbf{A}}$ on the other hand will give

$$\bar{A}_{i,j} = -\frac{\zeta^2}{2}\bar{B}_{i,j} + \zeta\delta_{i,j} - \bar{\chi}_{i,j}\,, \tag{3.7}$$

where $\bar{\chi}$ is the potential part of the $\bar{\mathbf{A}}$ matrix and is defined as

$$\bar{\chi}_{i,j} = \int_0^\infty \bar{\Phi}_i \frac{V(\gamma, r)}{r} \bar{\Phi}_j r^2 \,\mathrm{d}r\,. \tag{3.8}$$

Recurrence relations for generalized Laguerre polynomials utilized in $\bar{\Phi}_i$'s lead to the recursion

$$\bar{\chi}_{i+1,j} = [(i+1)(i+2l+2)]^{-1/2}\{[(j+1)(j+2l+2)]^{1/2}\bar{\chi}_{i,j+1}$$
$$+[j(j+2l+1)]^{1/2}\bar{\chi}_{i,j-1} - [i(i+2l+1)]^{1/2}\bar{\chi}_{i-1,j} + 2(i-j)\bar{\chi}_{i,j}\Big\}\,. \tag{3.9}$$

This is valid for all non-negative i, j and if any of the indices are negative, the corresponding $\bar{\chi}_{-1,j}$ (or $\bar{\chi}_{i,-1}$) should be taken as zero.

Once the zeroth row (or equivalently column) of $\bar{\chi}$ is known, the whole matrix

can be easily constructed via the recursive relation above. The nature of the recursion requires the computation of twice the number of row elements then what is otherwise needed from a direct evaluation of the matrix. However, this method is not only computationally less time consuming and more accurate but is also quite general for screening functions of similar nature if the same Laguerre basis set is employed. In other words, the formulation developed so far in evaluating the $\bar{\mathbf{A}}$ and $\bar{\mathbf{B}}$ matrices do not require a detailed knowledge of $V(\gamma, r)$ and is therefore reutilizable for potentials of similar nature. In short, it is integrals of the type

$$\bar{\chi}_{0,j} = \int_0^\infty \bar{\phi}_0 \frac{V(\gamma, r)}{r} \bar{\phi}_j r^2 \, \mathrm{d}r \tag{3.10}$$

that are to be further evaluated. For the Yukawa potential, they turn out to be

$$\bar{\chi}_{0,j} = \bar{\mathcal{N}}_0 \bar{\mathcal{N}}_j^{-1} \frac{1}{4\zeta^2} \frac{\bar{\gamma}^j}{(1+\bar{\gamma})^{j+2l+2}} , \tag{3.11}$$

where

$$\bar{\gamma} = \frac{\gamma}{2\zeta} . \tag{3.12}$$

To proceed with matrix elements of the type $A_{m,i}$ and $B_{m,i}$ it is worth noting that (3.2) will be utilized. Once again, it is more convenient to use $\bar{\phi}_i$'s rather than ϕ_i's. Therefore, it is matrix elements

$$\bar{A}_{m,i} = \int_0^\infty \Phi \mathcal{H} \bar{\phi}_i r^2 \, \mathrm{d}r \tag{3.13}$$

and

$$\bar{B}_{m,i} = \int_0^\infty \Phi \bar{\phi}_i r^2 \, \mathrm{d}r \tag{3.14}$$

that have to be calculated. Then the transformation (3.5) followed by the Gram–Schmidt procedure (2.18) will give the corresponding $A_{m,i}$ and $B_{m,i}$, the latter of which will yield a $\mathbf{B}$ matrix which will be the $(m+1) \times (m+1)$ unit matrix.

In evaluating the relevant integrals it is more convenient to rewrite Φ in terms of y instead of r.

$$\Phi = \bar{\mathcal{D}} \sum_{p=0}^{l} \frac{(l+p)!}{p!(l-p)!} (2\bar{\nu}y)^{l-p} \mathrm{e}^{-\bar{\nu}y} \frac{(1-\mathrm{e}^{-\bar{\mu}y})^{2l+1}}{y^{l+1}} . \tag{3.15}$$

The parameters $\bar{\nu}$ and $\bar{\mu}$ are defined as

$$\bar{\nu} = \frac{\nu}{2\zeta} , \tag{3.16}$$

$$\bar{\mu} = \frac{\mu}{2\zeta} , \tag{3.17}$$

and the new normalization constant $\bar{\mathcal{D}}$ absorbs all the relevant factors under the weight r^2.

The integrals in question can be easily evaluated by employing the explicit expression for the Laguerre polynomials [39] appearing in ϕ_i's and utilizing a binomial expansion for the last term in Φ. The relevant matrix element turn out to be

$$\bar{B}_{m,i} = (2\zeta)^{-3}\bar{\mathcal{D}}\bar{\mathcal{N}}_i \sum_{k=0}^{i}\sum_{p=0}^{l} \frac{(l+p)!}{(l-p)!p!}(2\bar{\nu})^{l-p}\frac{(-1)^k}{k!}\frac{(i+2l+1)!}{(k+2l+1)!(i-k)!}$$

$$\sum_{t=0}^{2l+1}\frac{(2l+1)!}{t!(2l+1-t)!}\frac{(l+k+1-p)!(-1)^t}{(\bar{\nu}+0.5+t\bar{\mu})^{l+k+2-p}}, \tag{3.18}$$

$$\bar{A}_{m,i} = \zeta^2\Bigg\{ -\tfrac{1}{2}\bar{B}_{m,i} + 2(i+l+1)(2\zeta)^{-3}\bar{\mathcal{D}}\mathcal{N}_i$$

$$\sum_{k=0}^{i}\sum_{p=0}^{l}\frac{(l+p)!}{(l-p)!p!}(2\bar{\nu})^{l-p}\frac{(-1)^k}{k!}\frac{(i+2l+1)!}{(k+2l+1)!(i-k)!}$$

$$\sum_{t=0}^{2l+1}\frac{(2l+1)!}{t!(2l+1-t)!}\frac{(l+k-p)!(-1)^t}{(\bar{\nu}+0.5+t\bar{\mu})^{l+k+1-p}}\Bigg\}$$

$$-(-2\zeta)^{-2}\bar{\mathcal{D}}\bar{\mathcal{N}}_i\sum_{k=0}^{i}\sum_{p=0}^{l}\frac{(l+p)!}{(l-p)!p!}(2\bar{\nu})^{l-p}\frac{(-1)^k}{k!}\frac{(i+2l+1)!}{(k+2l+1)!(i-k)!}$$

$$\sum_{t=0}^{2l+1}\frac{(2l+1)!}{t!(2l+1-t)!}\frac{(l+k-p)!(-1)^t}{(\bar{\nu}+0.5+t\bar{\mu}+\bar{\gamma})^{l+k+1-p}}. \tag{3.19}$$

Finally the matrix elements of the type $A_{m,m}$ and $B_{m,m}$ have to be calculated. To this end, the corresponding $\bar{\mathbf{A}}, \bar{\mathbf{B}}$ matrix elements

$$\bar{A}_{m,m} = \int_0^\infty \Phi\mathcal{H}\Phi r^2\,\mathrm{d}r \tag{3.20}$$

and

$$\bar{B}_{m,m} = \int_0^\infty \Phi\Phi r^2\,\mathrm{d}r \tag{3.21}$$

have to be calculated. Then the Gram–Schmidt procedure (2.18) is to be applied, giving the elements $A_{m,m}$ and $B_{m,m}$. Needless to say, since the function Φ is chosen to be normalized under the weight r^2

$$\bar{B}_{m,m} = 1\,. \tag{3.22}$$

On the other hand calculation of $\bar{A}_{m,m}$ is more difficult. To this end the following definition is made

$$\Omega_{s,t}(\tau,\eta) = \int_0^\infty \mathrm{e}^{-ry} \frac{(1-\mathrm{e}^{-\eta y})^s}{y^t} \mathrm{d}y \,. \tag{3.23}$$

The $\Omega_{s,t}(\tau,\eta)$ integrals to be utilized in matrix element $\bar{A}_{m,m}$ and in $\bar{\mathcal{D}}$ require that $s > t$. This leads to the recursive relation

$$\Omega_{s,t+1}(\tau,\eta) = \frac{s}{t}\eta\Omega_{s-1,t}(\tau,\eta) - \frac{\tau+s\eta}{t}\Omega_{s,t}(\tau,\eta) \tag{3.24}$$

valid for $t \geqslant 1$. To start the recursion, the equality

$$\Omega_{s,1}(\tau,\eta) = \sum_{k=0}^{s-1} \frac{s!(-1)^{s-k+1}}{(s-k)!k!} \ln(\tau+[s-k]\eta) - \ln\tau \tag{3.25}$$

is to be used. Now for the case when $t = 0$,

$$\Omega_{s,0}(\tau,\eta) = \sum_{k=0}^{s} \frac{s!(-1)^k}{(s-k)!k!} \frac{1}{(\tau+\eta k)} \,. \tag{3.26}$$

In terms of Ω integrals, $\bar{A}_{m,m}$ turns out to be

$$\begin{aligned}
\bar{A}_{m,m} = {} & \frac{\bar{\mathcal{D}}^2}{2\zeta} \sum_{p=0}^{l} \sum_{q=0}^{l} \frac{(l+p)!}{(l-p)!p!} \frac{(l+q)!}{(l-q)!q!} (2\bar{\nu})^{2l-p-q} \\
& \{\tfrac{1}{2}[\bar{\nu}+(2l+1)\bar{\mu}]^2 \Omega_{4l+2,p+q}(2\bar{\nu},\bar{\mu}) - (2l+1) \\
& \quad \times [\bar{\nu}+(2l+1)\bar{\mu}]\bar{\mu}\Omega_{4l+1,p+q}(2\bar{\nu},\bar{\mu}) \\
& + \tfrac{1}{2}(p+q+2)[\bar{\nu}+(2l+1)\bar{\mu}]\Omega_{4l+1,p+q+1}(2\bar{\nu},\bar{\mu}) \\
& + \tfrac{1}{2}(2l+1)^2\bar{\mu}^2\Omega_{4l,p+q}(2\bar{\nu},\bar{\mu}) \\
& - \tfrac{1}{2}(2l+1)\bar{\mu}(p+q+2)\Omega_{4l+1,p+q+1}(2\bar{\nu},\bar{\mu}) \\
& + \tfrac{1}{2}(p+1)(q+1)\Omega_{4l+2,p+q+2}(2\bar{\nu},\bar{\mu}) + \tfrac{1}{2}l(l+1)\Omega_{4l+2,p+q+2}(2\bar{\nu},\bar{\mu})\} \\
& - \frac{1}{4\zeta^2}\bar{\mathcal{D}}^2 \sum_{p=0}^{l} \sum_{q=0}^{l} \frac{(l+p)!}{(l-p)!p!} \frac{(l+q)!}{(l-q)!q!} (2\bar{\nu})^{2l-p-q} \Omega_{4l+2,p+q}(2\bar{\nu}+\bar{\gamma},\bar{\mu}) \,.
\end{aligned} \tag{3.27}$$

The normalization constant can be evaluated also in terms of the Ω integrals

$$\bar{\mathcal{D}} = \left\{ \frac{1}{8\zeta^3} \sum_{p=0}^{l} \sum_{q=0}^{l} \frac{(l+p)!}{(l-p)!p!} \frac{(l+q)!}{(l-q)!q!} (2\bar{\nu})^{2l-p-q} \Omega_{4l+2,p+q}(2\bar{\nu},\bar{\mu}) \right\}^{-1/2} \,. \tag{3.28}$$

4. Results

The afore-mentioned auto-coherent scheme is applied to calculate first few s, p, d states of the Yukawa potential system for several screening parameters from between the hydrogenic case and the threshold of continuum. As was previously mentioned, a starting v value (or equivalently an E value) is required for each specific γ value and state under consideration. In the cases where an easy estimation of the energy to be evaluated is not possible, a rule of thumb can be proposed. Take the converged energy value of the Yukawa system with a γ value closer to the hydrogenic limit and evaluate the corresponding v value. Calculate the corresponding eigenvalue of the variational matrix for a specific dimension. If the eigenvalue is negative then proceed with auto-coherency. If, on the other hand, it is positive then halve the energy estimate. Proceed with this until either the variational energy is negative or the halving process has been repeated to a prescribed number (in our case 7). If still a negative variational energy is not obtained then increase the dimension of the variational matrix by Δm and pick up the original energy estimate used in the beginning of the procedure for the previous dimension. Repeat this procedure until a negative value is obtained for the variational energy. When a negative variational energy is obtained for a specific dimension proceed with the auto-coherent scheme until self-consistency is achieved to within a previously prescribed ϵ tolerance (in our case often 1.0×10^{-30}, in worse cases 1.0×10^{-28}). Due to various factors such as accumulation of errors, ill-conditioned structures etc. the desired precision can never be reached within the given dimension. Hence the number of loops should be restricted to a pre-determined value (in our case 20). And somehow the situation should be recorded. In any case, if for a given dimension the variational or auto-coherent energy is negative the dimension is increased by Δm and the variational or auto-coherent energies for the two consecutive dimensions are checked to agree with each other to within an ϵ tolerance (in our case the two different tolerances were taken equal to each other) or if a pre-determined maximum variational dimension is reached. Then this situation is also recorded. The value of the maximum variational dimension is chosen with regards to certain properties of the computational medium such as machine precision and architecture. To save computational time the variational matrix elements corresponding to the maximum number of Laguerre basis functions are to be calculated once and for all and stored. For a given dimension the necessary matrix elements are taken from storage and only the terms corresponding to the extra function are reevaluated in the auto-coherent cycle. This attitude is obviously equally time-saving when dimension is increased.

Calculations were performed on a VAX/11-780 in Fortran 77 level quadruple precision arithmetic. Energy values calculated using the method presented here are given in tables 1–6. The first three tables include the results for the ground and the first two excited states of the spherically symmetric case. The remaining three tables correspond to the $l = 1$ and $l = 2$ values. In all of these six tables, special

Table 1
Calculated 1s energies (E) of the Yukawa potential for various screening parameter values (γ).

γ	E
0.1	−0.407 058 030 613 403 156 754 507 070 361
0.5	−0.148 117 021 889 932 616 711 758 220 725
1.0	−0.010 285 789 990 017 696 804 774 215 315
1.1	−0.002 287 244 234 053 485 463 476 080 685
1.19	−0.000 000 103 031 961 498 984 588 555 542
1.1906	−0.000 000 000 042 378 868 850 670 237 750
1.1906124	−0.000 000 000 000 000 121 835 370 047 917
1.190612421	−0.000 000 000 000 000 000 001 009 322 977
1.19061242106	−0.000 000 000 000 000 000 000 000 104 807
1.19061242106061	−0.000 000 000 000 000 000 000 000 000 016

Table 2
Calculated 2s energies (E) of the Yukawa potential for various screening parameter values (γ).

γ	E
0.1	−0.049 928 271 331 918 889 234 996 681 037
0.2	−0.012 107 865 195 440 464 385 855 372 409
0.3	−0.000 091 602 443 891 898 903 833 923 471
0.31	−0.000 000 037 992 565 724 034 305 218 565
0.3102	−0.000 000 000 074 725 279 816 856 888 985
0.3102092	−0.000 000 000 000 005 932 937 081 603 600
0.310209282	−0.000 000 000 000 000 000 442 009 920 526
0.31020928271	−0.000 000 000 000 000 000 000 013 440 942
0.3102092827139	−0.000 000 000 000 000 000 000 000 001 183
0.310209282713935	−0.000 000 000 000 000 000 000 000 000 003

Table 3
Calculated 3s energies (E) of the Yukawa potential for various screening parameter values (γ).

γ	E
0.05	−0.019 352 554 814 752 342 295 397 996 789
0.1	−0.003 208 046 744 690 258 718 213 516 794
0.13	−0.000 165 431 777 939 151 092 883 617 278
0.1394	−0.000 000 004 513 313 401 080 808 571 675
0.13945	−0.000 000 000 000 154 261 175 736 537 687
0.13945029	−0.000 000 000 000 000 029 465 737 439 451
0.139450294	−0.000 000 000 000 000 000 007 347 581 449
0.139450294064	−0.000 000 000 000 000 000 000 000 056 530
0.13945029406417	−0.000 000 000 000 000 000 000 000 000 115
0.139450294064177	−0.000 000 000 000 000 000 000 000 000 002

Table 4
Calculated 2p energies (E) of the Yukawa potential for various screening parameter values (γ).

γ	E
0.1	−0.046 534 390 486 724 608 386 600 840 395
0.2	−0.004 101 646 530 784 090 388 446 610 214
0.22	−0.000 028 697 244 985 229 882 829 234 829
0.220216	−0.000 000 101 948 775 845 390 353 568 20
0.220216806	−0.000 000 000 076 444 099 543 794 971 98
0.220216806606	−0.000 000 000 000 072 212 387 886 526 80
0.220216806606573	−0.000 000 000 000 000 005 091 678 061 43
0.22021680660657304	−0.000 000 000 000 000 000 051 041 667 52
0.220216806606573040405	−0.000 000 000 000 000 000 000 005 225 01
0.2202168066065730404050 41	−0.000 000 000 000 000 000 000 000 058 36

Table 5
Calculated 3p energies (E) of the Yukawa potential for various screening parameter values (γ).

γ	E
0.05	−0.018 557 751 883 405 996 604 893 993 884
0.1	−0.001 589 001 525 867 560 267 558 634 938
0.112	−0.000 050 088 397 121 471 206 121 055‘555
0.11271	−0.000 000 029 651 104 995 846 226 958 7
0.112710498	−0.000 000 000 021 296 705 343 614 794 6
0.112710498359	−0.000 000 000 000 031 091 836 861 286 2
0.112710498359524	−0.000 000 000 000 000 055 969 382 183 1
0.1127104983595249 44	−0.000 000 000 000 000 000 057 686 937 0
0.1127104983595249 44973	−0.000 000 000 000 000 000 000 057 626 5
0.1127104983595249 44973972	−0.000 000 000 000 000 000 000 000 056 4

Table 6
Calculated 3d energies (E) of the Yukawa potential for various screening parameter values (γ).

γ	E
0.05	−0.016 915 570 569 815 842 886 114 758 244
0.09	−0.000 312 913 502 634 921 634 216 385 5
0.091	−0.000 077 674 981 602 788 411 765 865 6
0.091345	−0.000 000 026 801 439 315 403 199 870 7
0.09134512	−0.000 000 000 171 260 371 731 456 283 3
0.091345120771	−0.000 000 000 000 162 484 163 019 785 1
0.091345120771732	−0.000 000 000 000 000 041 038 572 430 4
0.091345120771732184	−0.000 000 000 000 000 000 205 874 483 4
0.0913451207717321 84927	−0.000 000 000 000 000 000 000 157 575 7
0.0913451207717321 8492771	−0.000 000 000 000 000 000 000 000 014 9

emphasis is given to the critical γ region since this proved to be the most problematic part of the γ domain in various previous calculations [19,32,36]. However, few examples of lower lying γ's are also included to show the obvious validity of the method in the whole γ domain. Indeed the numerical results show that a non-negligible decrease in the variational dimension is observed even in the non-threshold regime when in addition to the Laguerre basis set an extra function is employed together with the proposed scheme. Although the choice of the parameter ν is quite apparent and has led to the utilization of an auto-coherent scheme, selection of the parameters ζ and μ are not so straightforward. The parameter ζ was in fact introduced for the sole purpose of convergence acceleration and can in principal be chosen as unity at the expense of fast convergence. However in the calculations, various reasonable ζ values were tested to increase the efficiency of the method. On the other hand choosing reasonable μ values is somewhat troublesome. Although μ is meant to be related to γ, the functional relation seems to be quite obscure since a preference to use only a single extra function was made to prevent overcomplicating the method. It was finally decided to utilize the trial and error approach in choosing values for μ.

The tables show that the method is capable of obtaining quite small energy values often to orders of 10^{-28}. The investigation of these threshold regimes implies that energy (E) becomes proportional to $(\gamma = \gamma_{cr})$ and the proportionality constant seems to be zero for s states when γ approaches γ_{cr}. In other words, energy seems to be expandable in positive powers of $(\gamma - \gamma_{cr})$. However the exact nature of such expansions awaits further research.

5. Concluding remarks

The extended basis set proposed, together with the auto-coherent scheme employed seems to be quite effective in determining the discrete spectra of the radial Schrödinger equation with Yukawa potential. The improvement is quite apparent in the region close to the threshold of the continuous spectrum. This is perhaps somewhat conceivable since the extra function has been selected such that it not only reflects the behavior of the problem at $r \to 0$ but also at $r \to \infty$. It is reassuring to see that the critical γ values given by Demiralp [37] agree perfectly with tables 1–6 of the present work.

The proposed scheme seems to be quite general for radially screened Coulomb potentials of the same nature. Obviously an appropriate extra function has to be employed for each specific case within the guidelines given in section 2. Work is in progress on linear combination of Yukawa functions and on Gaussian type functions as alternative examples to test the validity of the method.

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