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A BASIS SET COMPARISON IN A VARIATIONAL SCHEME FOR THE YUKAWA POTENTIAL

M. DEMIRALP
Department of Engineering Sciences, Faculty of Sciences and Letters,
Istanbul Technical University, Ayazağa Campus, 80626, Maslak-Istanbul, Turkey

N.A. BAYKARA and H. TAŞELI
Department of Mathematics, TÜBITAK, Marmara Research Center, P.O. Box 21,
41470 Gebze-Kocaeli, Turkey

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Abstract

The variational method is used to obtain solutions to Schrödinger's equation for a particle in the radially screened Yukawa potential. A basis set is presented. While the Laguerre basis set shows considerable improvement over the hydrogenic one, problems are still encountered as the screening parameter approaches its threshold value. Variational calculations are also presented using an Eckart-type basis set which looks promising near the critical screening region.

1. Introduction

Screened Coulomb potentials have received considerable interest among physical scientists since the early days of quantum mechanics. The most commonly used ones are those having spherical symmetry representing the presence of purely radial static screening.

In this paper, we shall deal with the Yukawa potential:

$$V(\gamma, r) = -\frac{e^{-\gamma r}}{r}, \tag{1.1}$$

where γ is a screening parameter. It arises in the solution of the Klein–Gordon equation for a static meson field [1,2]. It was also utilized in solid state [3,4] and plasma physics [5–9] and is known in the latter as the Debye–Hückel potential. In quantum chemistry, a linear combination of Yukawa or similar potentials can be used to model the effect of core electrons on the valence levels, thereby reducing the size of the calculations considerably. Since the Schrödinger equation employing the potential given by (1.1) is not analytically solvable, investigations have been carried out over the last couple of decades towards understanding and solving this problem, using various techniques. Variational [3,4,6,7,10–14], perturbational [6–8,11,12,15–22], group-theoretical [23–25] approaches, as well as numerical integration [26–31] and newly developed algebraic [32,33] methods have been utilized to this end.

The Schrödinger equation for a particle bound in a Yukawa potential is given by the following equation:

$$-\tfrac{1}{2}\nabla^2\Psi - \frac{e^{-\gamma r}}{r}\Psi = E\Psi; \qquad \Psi \in \mathcal{H}, \tag{1.2}$$

where $\mathcal{H}$ is the Hilbert space and r denotes the radial variable in spherical coordinates. As was previously stated, γ characterizes the screening of the central force field by other electrically charged particles. It is clear that for the problem at hand, the amplitude of the screening is independent of direction. One can therefore, after separation of variables, arrive at the corresponding radial form of (1.2):

$$-\frac{1}{2}\frac{d^2\psi}{dr^2} - \frac{1}{r}\frac{d\psi}{dr^2} + \left[\frac{l(l+1)}{2r^2} - \frac{e^{-\gamma r}}{r}\right]\psi = E\psi, \tag{1.3}$$

where ψ, the radial part of the wave function, depends on r and l ($=0, 1, 2, \ldots$) denotes the eigenvalues of the system's angular momentum operator. The boundary conditions accompanying (1.3) are the regularity, the continuity and the vanishing behaviour of ψ as r approaches infinity. It is clear that $V(0, r)$ is $-1/r$, that is, as the screening parameter and hence the screening goes to zero one is left with the radial Schrödinger equation of the hydrogen atom. It is perhaps this limiting behaviour of (1.3) that inspired considerable work using hydrogenic wave functions as bases for calculations.

Some of the more interesting variational calculations were done using the wave functions arising from the analytical solution of a Hulthen-like effective potential [11,14,34] as trial functions. In fact, the earlier of these works, which deals with only the s-states, uses also the perturbation technique. However, the quality of their perturbation results is inferior to that of their variational results, as screening increases.

It is well known by now that the presence of the continuum states complicates perturbation treatment of hydrogenic problems. An integration over the continuum would therefore be required for proper treatment of such problems. Perturbational methods which attempt to bypass this difficulty are logarithmic perturbation theory [18], Hellman–Feynman and hypervirial theorems [16], and a very recent perturbational treatment employing a Laguerre basis set expansion in the procedure to obtain the inversion of the hydrogen-like operator [20–22]. In a recent attempt to analyze the behaviour of the Padé approximants of ref. [17], Vrscay gives energy values to twenty decimal points for a sizeable screening domain for the 1s and 2s states with apparent loss of accuracy for large γ-values of the 2p state [19]. However, a multiple-precision floating-point arithmetic package was used to obtain these results and, moreover, the Stieltjes behaviour of the Padé series assumed by Lai proved to be false. This, of course, leaves open the question as to when and where the perturbation series of ref. [17] will converge.

In a recent perturbational scheme by the present authors, utilization of the Laguerre basis set in the inversion of the hydrogen-like operator has led to values consistent to thirty decimal points for a wide domain of the screening value. This approach does not seem to present extra convergence difficulties for states with l values greater than zero. At this stage, we have decided to carry out variational calculations with the Laguerre basis set and, for comparative purposes, to also perform calculations, within the same machine accuracy, using the hydrogenic basis set.

An alternative route to solving the Schrödinger equations with screened Coulomb potentials has been to approximate these potentials, as best one can, with other potentials which can be analytically solved. One such paper we find of considerable interest is that of Dutt et al. [35–37]. They approximate the Yukawa potential together with the angularly-dependent term of eq. (1.3) by an Eckart-type potential [38], extending the Ecker–Weizel [5] approximation to the non-zero angular momentum states. We find the closeness of their energies to Yukawa energies to be encouraging. Taking our cue from this work, we have decided to make variational calculations also employing such a basis set, for comparison.

In the light of the above discussions, a formulation of the variational scheme and matrix elements for various basis sets will be given in the next section. The third section will cover the results, while the final section will present the concluding results.

2. Formulation

The variational treatment of the eigenvalue equation (1.3) requires the selection of radial trial functions $\chi_{n,l}(\gamma, r)$ for a given state (n, l). Omitting the argument and the subscripts for the sake of convenience, and assuming the trial functions are normalized, that is,

$$\int_0^\infty \chi^* \chi r^2 \mathrm{d}r = 1, \tag{2.1}$$

the variational energy is expressible as

$$\overline{E} = \int_0^\infty \chi^* \left(-\frac{1}{2} \frac{\mathrm{d}^2 \chi}{2\mathrm{d}r^2} - \frac{1}{r} \frac{\mathrm{d}\chi}{\mathrm{d}r} + \left[\frac{l(l+1)}{2r^2} - \frac{\mathrm{e}^{-\gamma r}}{r} \right] \chi \right) r^2 \mathrm{d}r. \tag{2.2}$$

Taking the trial functions as linear combinations of known functions u will lead to the matrix eigenvalue problem:

$$\mathbf{A}\,\mathbf{C} = \overline{E}\,\mathbf{B}\,\mathbf{C}, \tag{2.3}$$

where

$$A_{i,j} = \int_0^\infty r^2 u_i \left(-\frac{1}{2}\frac{\mathrm{d}^2}{\mathrm{d}r^2} - \frac{1}{r}\frac{\mathrm{d}}{\mathrm{d}r} + \left[\frac{l(l+1)}{2r^2} - \frac{\mathrm{e}^{-\gamma r}}{r} \right] \right) u_j \mathrm{d}r, \tag{2.4}$$

$$B_{i,j} = \int_0^\infty u_i u_j r^2 \mathrm{d}r, \tag{2.5}$$

and the matrix $\mathbf{C}$ contains the coefficients of expansion. The symmetry constraints will allow the construction of a separate eigenvalue problem for each l value. Hence, the index i starting from zero will be expressible as

$$i = n - l - 1 \tag{2.6}$$

in terms of the usual quantum numbers n, l.

2.1. HYDROGENIC BASIS SET

An eigenfunction of a state denoted by (n, l) for a hydrogen-like system with nuclear charge ζ is expressible in terms of the associated Laguerre polynomials [39]:

$$u_i = N_i y^l \mathrm{e}^{-y/2} L_i^{2l+1}(y), \tag{2.7}$$

where

$$y = \frac{2\zeta r}{(i+l+1)} \tag{2.8}$$

and the normalization constant is given as [39]:

$$N_i = \frac{2}{(i+l+1)^2}\,\frac{1}{(i+2l+1)!}\left[\frac{i!}{(i+2l+1)!}\right]^{1/2} \zeta^{3/2}. \tag{2.9}$$

The well-known orthonormality of these functions under the weight r^2 will cause the weight matrix of eq. (2.3) to be a unit matrix, leading to the simpler diagonalization problem

$$\mathbf{A}\,\mathbf{C} = \overline{E}\,\mathbf{C}. \tag{2.10}$$

Expressing the elements of the matrix $\mathbf{A}$ as follows:

$$A_{i,j} = \int_0^\infty r^2 u_i \left(-\frac{1}{2} \frac{\mathrm{d}^2}{\mathrm{d}r^2} - \frac{1}{r} \frac{\mathrm{d}}{\mathrm{d}r} + \left[\frac{l(l+1)}{2r^2} - \frac{\zeta}{r} \right] \right) u_j \mathrm{d}r$$

$$+ \int_0^\infty u_i (\zeta - \mathrm{e}^{\gamma r}) u_j r \mathrm{d}r, \tag{2.11}$$

it is obvious that since u's are eigenfunctions of the operator appearing in the first term of eq. (2.11):

$$A_{i,j} = -\frac{\zeta^2}{2(i+l+1)^2} \delta_{i,j} \int_0^\infty u_i (\zeta - \mathrm{e}^{\gamma r}) u_j r \mathrm{d}r. \tag{2.12}$$

All that has to be done now is to calculate the integral containing the Yukawa potential. The Coulomb part of the integral can be calculated simply by setting γ equal to zero. Defining the quantities:

$$\lambda = (i+l+1)^{-1}, \tag{2.13}$$

$$\mu = (j+l+1)^{-1}, \tag{2.14}$$

$$\nu = (\lambda + \mu + \lambda / \zeta)/2, \tag{2.15}$$

$$\eta = \frac{\lambda}{(\nu - \lambda)} \frac{\mu}{(\nu - \mu)}, \tag{2.16}$$

the Yukawa potential can be evaluated to yield [41]:

$$\int_0^\infty u_i u_j \mathrm{e}^{\gamma r} r \mathrm{d}r = N_i N_j \frac{\lambda^l \mu^l}{(2\zeta)^2} \frac{(i+j+2l+1)!}{i!\,j!} \frac{(\nu - \lambda)^i (\nu - \mu)^j}{\nu^{i+j+2l+2}}$$

$${}_2F_1(-i, -j; -i-j-2l-1; 1-\eta), \tag{2.17}$$

where the function ${}_2F_1(a, b; c; z)$ is known in the literature as a hypergeometric function [39]. Since in this particular case the a and b value of the function are negative integers, it reduces to a finite sum and can be easily evaluated.

2.2. LAGUERRE BASIS SET

An alternative basis set which shall be employed in the present variational treatment is, in a sense, quite similar to (2.7):

$$u_1 = N_i y\, \mathrm{e}^{-y/2} L_i^{2l+1}(y). \tag{2.18}$$

Now, however,

$$y = 2\zeta r.$$

This set is orthonormal under the weight y, so that

$$N_i = \left[\frac{i!}{(i+2l+1)!}\right]^{1/2}. \tag{2.19}$$

The existence of Kronecker's deltas implies the weight matrix turns out to have a band structure,

$$B_{i,j} = (2\zeta)^{-3} N_i N_j \left[\frac{(i+2l+2)!}{i!}\delta_{i,j} + \frac{(i+2l+1)!}{(i-1)!}\delta_{i-1,j-1} - \frac{(i+2l+2)!}{i!}\delta_{i,j-1} - \frac{(i+2l+1)!}{(i-1)!}\delta_{i-1,j}\right]. \tag{2.20}$$

Employment of this basis set in eq. (2.4) will give

$$A_{i,j} = -(\zeta^2/2) B_{i,j} + \frac{(i+l+1)}{4\zeta}\delta_{i,j} - \int_0^\infty u_i u_j \mathrm{e}^{-\gamma r} r\, \mathrm{d}r. \tag{2.21}$$

To evaluate the Yukawa part of the A matrix, the following definition can be made:

$$D_{i,j} = \int_0^\infty u_i u_j \mathrm{e}^{-\gamma r} r\, \mathrm{d}r. \tag{2.22}$$

Using the recurrence formulae for Laguerre polynomials [39], a two-dimensional recursion relationship can be obtained [22]:

$$\begin{aligned} D_{i+1,j} = {} & [(i+1)(i+2l+2)]^{-1/2}\Big([(j+1)(i+2l+2)]^{1/2} D_{i,j+1} \\ & + [(j+1)(i+2l+1)]^{1/2} D_{i,j-1} - [(i+1)(i+2l+1)]^{1/2} D_{i-1,j} \\ & + 2(i-j) D_{i,j}\Big) \qquad i,j = 0,1,2,\dots . \end{aligned} \tag{2.23}$$

To start using this recurrence, all that needs to be done is to calculate the zeroth row (or equivalently, column) of D, which can be easily evaluated as

$$D_{0,j} = N_0 N_j^{-1} (2\zeta)^{-2} \frac{\bar{\gamma}^j}{(1+\bar{\gamma})^{j+2l+2}}, \tag{2.24}$$

where

$$\bar{\gamma} = \gamma/(2\zeta). \tag{2.25}$$

This leaves one with the evaluation of the eigenvalue problem of (2.3).

An equivalent choice is to consider

$$u_i = N_i y^l e^{-y/2} L_i^{2l+2}(y). \tag{2.26}$$

Again,

$$y = 2\zeta r, \tag{2.27}$$

and the set is orthonormal under the weight y^2, with

$$N_i = \left[\frac{i!}{(i+2l+2)!}\right]^{1/2}. \tag{2.28}$$

The utilization of (2.26) will result in time economy, computationally speaking, since it requires solving the unweighted problem of eq. (2.9). These two Laguerre bases are equivalent and a well-known relationship between them [39] can be used to obtain a transformation from the $(2l+1)$ to the $(2l+2)$ set

$$L_i^{\alpha+1}(y) = \sum_{k=0}^{i} L_k^{\alpha}(y). \tag{2.29}$$

2.3. ECKART-TYPE BASIS SET

The definition

$$u_i = f_i / r \tag{2.30}$$

leads to the eigenvalue problem of the form

$$\left(-\frac{1}{2}\frac{d^2}{dr^2} + \left[\frac{l(l+1)}{2r^2} - \frac{e^{-\gamma r}}{r}\right]\right) f_i = \bar{E} f_i. \tag{2.31}$$

Defining

$$y = (2e^{-\zeta r} - 1), \tag{2.32}$$

the trial functions will be chosen as

$$f_i = N_i \frac{(1+y)^{\nu}(1-y)^{l+1}}{2^{l+1+\nu}} P_i^{(2l+1,2\nu)}(y), \tag{2.33}$$

where $P_i^{(\alpha,\beta)}(y)$ is a Jacobi polynomial [39] and N_i is a parameter, arbitrarily chosen. This set will be chosen to be normalized under weight 1, so that:

$$N_i = \left[\frac{i!\,\Gamma(i+2\nu+2l+2)}{\Gamma(i+2l+1)\Gamma(i+2\nu+1)} (2i+2\nu+2l+2) \right]^{1/2}. \tag{2.34}$$

The weight matrix elements are

$$B_{i,j} = \frac{1}{\zeta} N_i N_j \int_{-1}^{+1} \frac{f_i(y) f_j(y)}{(1+y)}\, \mathrm{d}y, \tag{2.35}$$

and the corresponding Hamiltonian matrix elements are

$$\begin{aligned} A_{i,j} = {} & -\frac{\zeta^2}{2} B_{i,j} - \frac{\zeta^2}{2} l(l+1) N_i N_j \int_{-1}^{+1} \frac{f_i(y) f_j(y)}{(1-y)^2} (1+y)\mathrm{d}y \\ & - \frac{\zeta}{2} [(j+\nu+l+1)^2 - \nu^2 - (l+1)] N_i N_j \int_{-1}^{+1} \frac{f_i(y) f_j(y)}{(1-y)} \mathrm{d}y \\ & + \frac{\zeta}{2} [(l(l+1)] N_i N_j \int_{-1}^{+1} \frac{f_i(y) f_j(y)}{(1+y)\ln^2([1+y]/2)} \mathrm{d}y \\ & + \frac{1}{2^{\bar{\gamma}}} N_i N_j \int_{-1}^{+1} \frac{f_i(y) f_j(y)}{(1-y)^{1-\bar{\gamma}} \ln[1+y]/2)} \mathrm{d}y, \end{aligned} \tag{2.36}$$

where

$$\bar{\gamma} = \gamma/\zeta. \tag{2.37}$$

Using the recurrence formulae for Jacobi polynomials [39] leads to a two-dimensional recursion relationship [22] similar in form to that of the Laguerre basis set. To start using such a recurrence, all that needs to be done is to calculate the zeroth row (or column) of the individual integrals appearing in eqs. (2.35) and (2.36).

An alternative route is to expand the Jacobi polynomials in terms of their argument

$$P_i^{(\alpha,\beta)}(y) = 2^{-N} \sum_{k=0}^{i} \binom{i+\alpha}{k} \binom{i+\beta}{i-k} (y+1)^k (y-1)^{i-k} \tag{2.38}$$

and integrate the individual integrals.

We have decided to use the latter route to prevent error accumulations. The final formulation is, however, quite long and rather tedious. Since this basis set is not within the main scope of this paper, we shall restrict ourselves to only a rather preliminary investigation and hence will not elaborate any further on the calculation of the Hamiltonian matrix elements.

3. Results

Numerical calculations have been carried out for all of the three aforementioned basis sets. To this end, a VAX-780 was employed, and programmes were executed in quadruple precision arithmetic.

Table 1

Rate of convergence of variational scheme using a hydrogenic basis set as a function of the order M for the 1s state.

M	$\gamma = 0.005$	$\gamma = 0.1$	$\gamma = 0.5$	$\gamma = 1.0$
1	- 0.4950 18687694	- 0.407029	- 0.140000	0.055555
2	- 0.4950 18687822	- 0.407045	- 0.145457	- 0.007767
3	- 0.4950 18687843	- 0.407047	- 0.145999	- 0.008151
4	- 0.4950 18687850	- 0.407048	- 0.146176	- 0.008287
5	- 0.4950 18687854	- 0.407048764	- 0.146258	- 0.008311
...	...	...	...	...
10	- 0.4950 18687858	- 0.407049335	- 0.146366	- 0.008349
15	- 0.4950 18687859	- 0.407049447	- 0.146387	- 0.008357
20	- 0.4950 18687859	- 0.407049487	- 0.146395	- 0.008360

Table 2

Rate of convergence of variational scheme using a hydrogenic basis set as a function of the order M for the 2s state.

M	$\gamma = 0.005$	$\gamma = 0.1$	$\gamma = 0.15$	$\gamma = 1.0$
2	- 0.120074 133392	- 0.081702	- 0.024300	0.010
3	- 0.120074 140708	- 0.081753	- 0.026915	- 0.002
4	- 0.120074 141696	- 0.081760	- 0.027012	- 0.003206
5	- 0.120074 142024	- 0.081762	- 0.027047	- 0.003268
...	...	...	...	...
10	- 0.120074 142371	- 0.081764503	- 0.027084	- 0.003280
15	- 0.120074 142427	- 0.081764871	- 0.027090	- 0.003280
20	- 0.120074 142447	- 0.081764998	- 0.027092	- 0.003284

In tables 1 and 2, the ground and first excited states are consecutively given as examples to the convergence rate of the Yukawa system when the hydrogenic set is employed as a basis. A reasonable selection of the screening parameter γ is given for both of these states. As for the size of truncation M, 1–5, 10, 15 and 20 are quoted to give a general feeling for what is a very slow convergence and is believed to be due to the non-existence of the contributions coming from the continuous spectrum eigenfunctions in the trial functions. No attempt was made to optimize any charge parameter; i.e. $\zeta = 1$ was employed, since detailed work using various ζ's already exists in the literature for small M values [7] and a more complete analysis would have been but a diversion from the main scheme of this work. For accurate energy values, tables 1 and 2 of ref. [22] and table 3 of the present work can be referred to.

Table 3

Variational energy eigenvalues for various states calculated using the Laguerre basis set as a function of γ.

State	γ	M	Energy
4f	0.045	50	– 0.001 487 359 743 334 720 048 551 730 070
4d	0.05	55	– 0.001 580 871 626 871 004 952 883 948 070
4p	0.05	55	– 0.002 598 058 852 571 853 965 261 191 255
4s	0.05	55	– 0.003 091 659 900 161 321 484 658 950 292
3d	0.05	35	– 0.016 915 570 569 815 842 886 114 758 244
3p	0.05	40	– 0.018 557 751 883 405 996 604 893 993 884
3p	0.1	70	– 0.001 589 001 525 867 560 267 558 634 938
3s	0.05	40	– 0.019 352 554 814 752 342 295 397 996 789
2p	0.1	35	– 0.046 534 390 486 724 608 383 600 840 395
2p	0.15	40	– 0.021 104 888 927 736 242 916 943 382 961
2p	0.2	65	– 0.004 101 646 530 784 090 388 446 910 214
2s	0.005	10	– 0.120 074 143 345 598 522 611 020 393 630
2s	0.05	25	– 0.081 771 195 795 253 124 173 489 413 770
2s	0.15	45	– 0.027 222 190 725 688 518 250 187 267 589
2s	0.25	70	– 0.003 395 906 283 239 307 796 442 264 449
1s	0.005	8	– 0.495 018 687 925 632 530 667 468 329 152
1s	0.1	20	– 0,407 058 030 613 403 156 754 507 070 361
1s	0.5	50	– 0.148 117 021 889 932 616 711 758 220 725
1s	1.0	85	– 0.010 285 789 990 017 696 804 774 214

In table 3, energy values evaluated using the Laguerre basis set are given. To be reasonably concise, only a few examples are presented, and all in the same table. In the first column are the symbols 1s, 2s, 2p, 3p, 3d, 4s, 4d and 4f, the states for which calculations have been made. The screening parameter γ, in the second column, has been varied over an important portion of its domain between threshold and zero. In the third column is given the size of truncation M necessary to obtain the quoted accuracy. The effective charge parameter γ turns out to be the same as those given in the previous perturbational treatment [22] and is therefore not employed in table 3. The last column is devoted to the presentation of our results corresponding to the state γ, M and ζ. Results are as good as those obtained via the perturbational scheme of ref. [22] and closer to the critical region, where the eigenvalues are close to the threshold of the continuous spectrum; the results are even much better, as can be noted for example for the 1s states $\gamma = 1.0$, where an additional five digit accuracy has been achieved. The most obvious advantages of variational calculations over the perturbational treatment of ref. [22] are the economy in computational time and that for former is less susceptible to error accumulations. Nevertheless, as γ approaches its critical value the variational method using the Laguerre basis set starts to lose its efficiency. This possibly seems to hint at the inappropriateness of the structure of the Laguerres for the problem at hand when heavy screening effects exist. This suggests considering basis functions arising from a problem of similar structure.

Table 4

Convergence rate of variational scheme using an Eckart-type basis set as a function of the order M for the 1s state.

M	$\gamma = 0.5$	$\gamma = 1.0$	$\gamma = 1.15$	$\gamma = 1.19$
5	– 0.148 1 1698 1639	– 0.010285232192	– 0.00045500	0.0000000
10	– 0.148 1 1702 1584	– 0.010285577292	– 0.00045525	0.0000000
15	– 0.148 1 1702 1890	– 0.010285789204	– 0.00045538	0.0000000
20	– 0.148 1 1702 1890	– 0.010285789990	– 0.00045588	– 0.0000001

Table 5

Convergence rate of variational scheme using an Eckart-type basis set as a function of the order M for the 2s state.

M	$\gamma = 0.15$	$\gamma = 0.25$	$\gamma = 0.30$	$\gamma = 0.31$
5	– 0.027222 188449	– 0.003395899984	– 0.00009 159	0.00000001
10	– 0.027222 190726	– 0.003395904486	– 0.00009 160	0.00000000
15	– 0.027222 190726	– 0.003395906134	– 0.00009 160	0.00000004
20	– 0.027222 190726	– 0.003395906283	– 0.00009 160	– 0.00000004

In tables 4 and 5, the ground and first excited states are consecutively given as examples to the convergence rate of the Yukawa system when the Eckart-type set is employed as a basis. The size of the truncation M, 5, 10, 15 and 20, is quoted to give a general feeling about the rate of convergence when this basis set is used. A specific selection of the screening parameter γ is made for both of these states, with special emphasis on values close to the threshold. The NAG Library routine E04CCF was utilized to optimize energies with respect to parameters γ and ν. Although the calculations to solve the eigenvalue problem were performed in quadruple precision arithmetic to prevent error accumulations, optimizations were done in double precision since all available NAG routines were implicitly so. It is worth noting that this is a rather costly process and is in no way an ultimate goal. All in all though, the expectations are at least partially fulfilled and results accurate to eight decimal points are, for example, calculated for the 2s state $\gamma = 0.31$. This would have been quite unlikely with either of the two aforementioned bases. For these γ values close to threshold, energies were checked with the results of tables 4 and 5 to the accuracy given in these tables. Although Vrscay's results are more accurate, the precision required seems to be much higher.

4. Conclusion and remarks

In this work, we have presented variational results for the Yukawa potential using Laguerre polynomials to form a basis set. The convergence rate is incomparably better than that of the hydrogenic basis set. This can be easily attributed to the different nature of the H-atom and the Yukawa problems. In the former, infinitely many discrete states exist, whereas in the latter, as soon as screening is introduced, the number of states becomes finite. That is, there is a critical γ for each state beyond which that particular state can not survive. The Laguerre polynomial results are slightly better than the perturbational results of the present authors [22], and are almost likewise troublesome on a narrow γ domain around the critical value of the screening parameter. For the low-lying states, at least for those that are given in refs. [19,22], the variational treatment of the problem using Laguerre polynomials is preferable to the perturbational treatment [22], since numerical results are less time-consuming and less susceptible to error accumulations. In the neighbourhood of the critical value, the present work gives better results although, especially for the s-states, they are lower in accuracy than Vrscay's results [19].

In this work, energy values evaluated using the Eckart-type basis set are also given. In the vicinity of the threshold, this basis set seems to be more appropriate than the Laguerre basis set. At the moment, however, calculations with this basis set require the optimization of parameters ζ and μ, which makes them somewhat cumbersome, time consuming and inadequate in accuracy.

To conclude, this work has been quite helpful in pointing out in which parts of the γ domain the different basis sets give better results, and also demonstrates the need to use this knowledge to try to construct new basis sets which will hopefully work in the whole domain. Work is in progress towards this aim. As a matter of fact, γ-threshold value calculations of a Yukawa-type potential were presented by using a similar type of basis function in a variational scheme [42].

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