Modified Laguerre Basis for Hydrogen-like Systems

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ABSTRACT: *N*-dimensional Schrödinger equation with isotropic nonpolynomial perturbations is studied. A Laguerre basis, which is different from that of the hydrogen atom in nature, has been introduced and applied to screened Coulomb potentials. Certain very useful recurrence relations are developed for the evaluation of matrix elements analytically. Specimen eigenvalue calculations to illustrate the method as well as its extension to other potentials are presented. © 1997 John Wiley & Sons, Inc. Int J Quant Chem **63:** 949–959, 1997

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1. Introduction

The radial form of the Schrödinger equation in N dimensions

$$\left[-\frac{1}{2}\frac{d^2}{dr^2}-\frac{N-1}{2r}\frac{d}{dr}+\frac{l(l+N-2)}{2r^2}+V(r)\right]\mathscr{R}(r)=E\mathscr{R}(r),\qquad \mathscr{R}\in L_2(0,\infty) \tag{1.1}$$

with a screened Coulomb potential has been the subject of many computational methods, where L_2 is the Hilbert space of the square integrable functions in the semi-infinite interval of r, $r\in[0,\infty)$. In this article, we mainly deal with such a potential which behaves like $-1/r$ as $r\to 0$ and vanishes at infinity. In particular, the Yukawa potential,

$$V(r)=-\frac{Z}{r}e^{-\gamma r},\qquad \gamma>0 \tag{1.2}$$

with the screening parameter γ and the exponential cosine screened Coulomb potential

$$V(r)=-\frac{Z}{r}e^{-\gamma r}\cos\lambda r \tag{1.3}$$

with the two parameters γ and λ are the most studied systems of this kind. In (1.2) and (1.3) Z stands for the nuclear charge, which can be made unity by a simple scaling transformation.

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The screened Coulomb potentials are of significant importance in atomic, plasma, and solid-state physics. In quantum chemistry, a linear combination of like potentials can be used to model the effect of core electrons on the valence levels. Therefore the Schrödinger equation in three dimensions, i.e., $N = 3$ in (1.1), employing those potentials was investigated with considerable intensity in the last decades [1–17]. More specifically, the Yukawa potential has been treated by perturbation theory and resummation techniques such as Pade approximants [1, 2], by convergent Rayleigh–Schrödinger perturbation series [3, 4], by a scaling variational scheme [5, 6], by the Ecker–Weizel approximation [7], by a unified power series–Hill determinant approach [8], by a renormalized hypervirial perturbative method [9], and by various numerical algorithms [10–12]. Some of these procedures [8, 9, 13–15] as well as a dynamical group approach and an algebraic perturbation theory [16, 17] have been applied to the exponential cosine screened Coulomb potential in (1.3).

The wave function $\mathscr{R}(r)$ in (1.1) should behave like r^l as $r \to 0$ since the potential $V(r)$ grows no faster than $1/r$ at the origin. Therefore, transforming the dependent variable from $\mathscr{R}(r)$ to $\Phi(r)$,

$$\mathscr{R}(r) = r^l \Phi(r), \tag{1.4}$$

it follows that

$$\left[-r\frac{d^2}{dr^2} - \alpha\frac{d}{dr} + 2rV(r)\right]\Phi(r) = 2rE\Phi(r), \tag{1.5}$$

which avoids the use of the term proportional to $1/r^2$ [18]. Here, we have defined a generalized angular momentum α,

$$\alpha = 2l + N - 1, \tag{1.6}$$

depending on both the angular momentum l and the space dimension N. It is shown, from (1.5), that the spectrum of the eigenvalue problem remains unchanged for a prescribed value of the sum $2l + N$. Hence the eigenvalues in N dimensions, denoted by $E^{(N)}_{n_r,l}$ with the radial and angular quantum numbers n_r and l, are degenerate in such a way that

$$\begin{aligned} E^{(2)}_{n_r,1} &\equiv E^{(4)}_{n_r,0} \\ E^{(2)}_{n_r,2} &\equiv E^{(4)}_{n_r,1} \equiv E^{(6)}_{n_r,0} \\ &\vdots \\ E^{(2)}_{n_r,l} &\equiv E^{(4)}_{n_r,l-1} \equiv E^{(6)}_{n_r,l-2} \equiv \cdots \equiv E^{(2l-2)}_{n_r,2} \\ &\equiv E^{(2l)}_{n_r,1} \equiv E^{(2l+2)}_{n_r,0} \end{aligned} \tag{1.7}$$

when N is even, where $E^{(2)}_{n_r,0}$ is single in the system. Likewise, if N is odd, then

$$\begin{aligned} E^{(3)}_{n_r,1} &\equiv E^{(5)}_{n_r,0} \\ E^{(3)}_{n_r,2} &\equiv E^{(5)}_{n_r,1} \equiv E^{(7)}_{n_r,0} \\ &\vdots \\ E^{(3)}_{n_r,l} &\equiv E^{(5)}_{n_r,l-1} \equiv E^{(7)}_{n_r,l-2} \equiv \cdots \equiv E^{(2l-1)}_{n_r,2} \\ &\equiv E^{(2l+1)}_{n_r,1} \equiv E^{(2l+3)}_{n_r,0} \end{aligned} \tag{1.8}$$

with $E^{(3)}_{n_r,0}$ which is equivalent to the antisymmetric state eigenvalues of the relevant one-dimensional equation. The degenerate structure of the spectrum of N-dimensional Schrödinger equation expressed by (1.7) and (1.8) now suggests evidently that we may consider only two- and three-dimensional cases, without any loss of generality.

The decaying behavior of the screened Coulomb potentials implies another characteristic property of (1.1) or (1.5) that E will have both continuous and discrete spectra. Furthermore, the problem yields a finite number of discrete eigenvalues provided that the screening parameters γ and λ are nonzero. It is well known that the case of $\gamma = \lambda = 0$ corresponds to the electronic Schrödinger equation for a hydrogen atom, which is solvable analytically giving a countably infinite discrete states. It is perhaps this special case of (1.1) that inspired developing several works based on the use of hydrogenic wave functions. However, the expansion of the wave function in terms of the discrete eigenfunctions of the hydrogen atom shows dramatically slow convergence properties due to the nonexistence of the contributions coming from the continuous spectrum eigendistributions [6]. The consideration of the uncountable infinite set of eigendistributions corresponding to the continuous spectrum, on the other hand, creates many technical problems. To overcome this situation it is preferable to seek an appropriate way of dealing with an operator, which possesses solely a discrete spectrum with a complete set of eigenfunctions, instead of the Hamiltonian for the hydrogen atom.

In fact, there are excellent studies on how the problem of the continuous spectrum can be bypassed [19–22]. Especially, the "$so(4, 2)$ Lie algebra

technology,'' which consists of the operators T_1, T_2, and T_3 satisfying certain commutation relations, reformulates hydrogenic problems over discrete Sturmian basis [19–21]. Before the developments of the $so(4,2)$ algebra, Löwdin and Shull had introduced an entirely discrete basis for performing various calculations on helium [23]. In Section 2, the required basis set is constructed in terms of the Laguerre functions, and its connections with the existing ones are given. The Rayleigh–Ritz variational calculations are carried out in Section 3 for the bound states of hydrogen-like atoms in a screened Coulomb potential field. The last section contains the conclusions and the motivation for extending the method to other systems, including Morse and Gaussian-type interactions.

2. Laguerre Basis Set

Rewriting Eq. (1.5) in the form

$$[T + 2rV(r)]\Phi(r) = 2r(E + \tfrac{1}{8})\Phi(r) \quad (2.1)$$

with

$$T = -r\frac{d^2}{dr^2} - \alpha\frac{d}{dr} + \frac{1}{4}r, \qquad \lim_{r\to\infty}\Phi(r) = 0, \quad (2.2)$$

we may see that the operator T has purely a discrete spectrum corresponding to a complete sequence of eigenfunctions:

$$\phi_n^{(\alpha-1)}(r) = \mathcal{N}_n^{(\alpha-1)} e^{-(1/2)r} L_n^{(\alpha-1)}(r), \qquad n = 0, 1, 2, \ldots, \quad (2.3)$$

where the $L_n^{(\alpha-1)}(r)$ are the associated Laguerre polynomials, $\mathcal{N}_n^{(\alpha-1)}$ is some normalization constant, and

$$T\phi_n^{(\alpha-1)}(r) = (n + \tfrac{1}{2}\alpha)\phi_n^{(\alpha-1)}(r). \quad (2.4)$$

In general, if the normalization constant is specified by the formula

$$\mathcal{N}_n^{(p)} = \sqrt{n!/\Gamma(n+p+1)}, \quad (2.5)$$

then the Laguerre functions $\phi_n^{(p)}(r)$ become orthonormal relative to the weighting function r^p over the interval of r, satisfying the asymptotic boundary condition at infinity. Thus we have

$$\int_0^\infty r^p \phi_m^{(p)}(r)\phi_n^{(p)}(r)\,dr = \delta_{mn}, \quad (2.6)$$

where δ_{mn} is the Kronecker delta.

It may be shown that the Laguerre basis set so defined is quite similar to the hydrogenic one in form but has different spectral properties. In our previous communications [3, 4], the operator T was regarded as the unperturbed operator in a Rayleigh–Schrödinger perturbation method. So the present article will be another version of showing the performance of this basis in the Rayleigh–Ritz variational picture. Moreover, the operator T is closely related to the operator T_3 appearing in the Lie algebra $so(2,1)$ for radial problems [19]. Actually, the so-called Sturmian basis associated with the T_3 operator can be reproduced from (2.3) if n and r are replaced by $n - l - 1$ and $2r$, respectively, for $N = 3$.

Now, postulating the wave function $\Phi(r)$ as the linear combination of the $\phi_n^{(\alpha-1)}(r)$ leads to the generalized matrix eigenvalue problem

$$\mathbf{Ac} = 2(E + \tfrac{1}{8})\mathbf{Bc}, \quad (2.7)$$

where

$$A_{mn} = (n + \tfrac{1}{2}\alpha)\delta_{mn} + 2\int_0^\infty r^\alpha V(r)\phi_m^{(\alpha-1)}(r)\phi_n^{(\alpha-1)}(r)\,dr \quad (2.8)$$

and

$$B_{mn} = \int_0^\infty r^\alpha \phi_m^{(\alpha-1)}(r)\phi_n^{(\alpha-1)}(r)\,dr \quad (2.9)$$

within the vector $\mathbf{c}$ containing the expansion coefficients. From the recurrence relation

$$L_m^{(p-1)}(r) = L_m^{(p)}(r) - L_{m-1}^{(p)}(r) \quad (2.10)$$

for the Laguerre polynomials [24], we find that the weight or overlap matrix $\mathbf{B}$ has the tridiagonal form,

$$B_{mn} = \frac{\mathcal{N}_n^{(\alpha-1)}}{\mathcal{N}_m^{(\alpha-1)}}[(2m + \alpha)\delta_{mn} - (m + \alpha)\delta_{m,n-1} - m\delta_{m-1,n}]. \quad (2.11)$$

In spite of this simple banded structure of $\mathbf{B}$ it is more convenient to cope with an unweighted

matrix eigenvalue problem. Since the set

$$\Big\{ e^{-(1/2)r} L_0^{(\alpha-1)}(r),\ e^{-(1/2)r} \times \big[L_0^{(\alpha-1)}(r) + L_1^{(\alpha-1)}(r) \big], \ldots, e^{-(1/2)r} \times \sum_{k=0}^{n} L_k^{(\alpha-1)}(r), \ldots \Big\} \tag{2.12}$$

obtained from (2.3) comprises also a basis of $L_2(0,\infty)$, on recalling the identity [24]

$$\sum_{k=0}^{n} L_k^{(p-1)}(r) = L_n^{(p)}(r), \tag{2.13}$$

we see that the functions

$$\phi_n^{(\alpha)}(r) = \mathscr{N}_n^{(\alpha)} e^{-(1/2)r} L_n^{(\alpha)}(r), \qquad n = 0, 1, 2, \ldots \tag{2.14}$$

are now orthonormal with respect to r^α. In three-dimensional case, $N = 3$, this basis set may also be derived from the radial part of the Löwdin–Shull basis on setting the adjustable parameter η therein as $\frac{1}{2}$ and replacing n by $n + l + 1$ [23]. As a result, interchanging $\phi_n^{(\alpha-1)}(r)$ in the above formulas by $\phi_n^{(\alpha)}(r)$, the weight matrix $\mathbf{B}$ is reduced to the identity matrix. In fact, two Laguerre basis in (2.3) and (2.14) are equivalent; however, the latter yields a standard matrix eigenvalue problem

$$\mathbf{Hc} = 2(E + \tfrac{1}{8})\mathbf{c}, \tag{2.15}$$

which makes a considerable simplification in the numerical computations, where

$$H_{mn} = \int_0^\infty r^{\alpha-1} \phi_m^{(\alpha)}(r) \big[T\phi_n^{(\alpha)}(r) \big]\, dr + 2\int_0^\infty r^\alpha V(r) \phi_m^{(\alpha)}(r) \phi_n^{(\alpha)}(r)\, dr. \tag{2.16}$$

Note that $\mathbf{H}$ and $\mathbf{B}^{-1}\mathbf{A}$ are similar matrices having the same eigenvalues so that, in a sense, we have defined the inverse of $\mathbf{B}$ by employing the connection between (2.3) and (2.14).

The integrals in the symmetrical variational matrix $\mathbf{H}$ are denoted by D_{mn} and V_{mn}, respectively, to write

$$H_{mn} = D_{mn} + V_{mn}. \tag{2.17}$$

The first integral can be evaluated explicitly, after some algebra, to give

$$D_{mn} = \mathscr{N}_m^{(\alpha)} \mathscr{N}_n^{(\alpha)} \sum_{k=0}^{K} \left(\frac{k + \alpha/2}{k + \alpha} \right) \big[\mathscr{N}_k^{(\alpha)} \big]^{-2}, \tag{2.18}$$

where the upper limit K of the summation is equal to $\mathrm{Min}(m, n)$, i.e., the smaller one of the indices m and n. Furthermore, the second integral V_{mn} containing the potential function may be shown to obey a recurrence relation. To this end, we use the identity for the Laguerre polynomials [24],

$$(n+1) L_{n+1}^{(p)}(r) - (2n + p + 1 - r) L_n^{(p)}(r) + (n + p) L_{n-1}^{(p)}(r) = 0 \tag{2.19}$$

to obtain a functional relation, for the product of two Laguerre functions, of the form

$$\begin{aligned} &\sqrt{(m+1)(m+p+1)}\ \phi_{m+1}^{(p)} \phi_n^{(p)} - 2(m-n)\phi_m^{(p)}\phi_n^{(p)} - \sqrt{n(n+p)}\ \phi_m^{(p)}\phi_{n-1}^{(p)} \\ &- \sqrt{(n+1)(n+p+1)}\ \phi_m^{(p)}\phi_{n+1}^{(p)} + \sqrt{m(m+p)}\ \phi_{m-1}^{(p)}\phi_n^{(p)} = 0, \end{aligned} \tag{2.20}$$

which implies immediately that

$$\begin{aligned} V_{m+1,n} = {} & \frac{1}{\sqrt{(m+1)(m+\alpha+1)}} \\ & \times \Big[\sqrt{(n+1)(n+\alpha+1)}\ V_{m,n+1} + 2(m-n) V_{m,n} + \sqrt{n(n+\alpha)}\ V_{m,n-1} \\ & - \sqrt{m(m+\alpha)}\ V_{m-1,n} \Big] \end{aligned} \tag{2.21}$$

for $m, n = 1, 2, \ldots,$ and

$$V_{1,n} = \frac{1}{\sqrt{\alpha+1}} \Big[\sqrt{(n+1)(n+\alpha+1)}\ V_{0,n+1} - 2nV_{0,n} + \sqrt{n(n+\alpha)}\ V_{0,n-1} \Big] \tag{2.22}$$

for $n = 1, 2, \ldots$. It is noteworthy that these relations of determining the first and the following rows of V_{mn} in turn are independent of the particular form of the potential function. To start using the recursions all that needs to be done is the calculation of the zeroth row (or column) entries

$$V_{0,n} = 2\int_0^\infty r^\alpha V(r) \phi_0^{(\alpha)}(r) \phi_n^{(\alpha)}(r)\, dr, \qquad V_{n,0} = V_{0,n}, \qquad n = 0, 1, \ldots \tag{2.23}$$

which is required as an initial condition for (2.21) and (2.22). Moreover, the labor involved in such a construction of the matrix may be considerably shortened by exploiting the symmetry, $V_{mn} = V_{nm}$.

3. Numerical Applications to Screened Coulomb Potentials

At the numerical side of this work, we assume the truncated wave function

$$\Phi(r) = \sum_{m=0}^{M-1} c_m \phi_m^{(\alpha)}(r), \tag{3.1}$$

leading to the diagonalization problem of a variational matrix of finite order. In this case, a knowledge of $2M - 1$ integrals defined by (2.23) over a prescribed potential function is sufficient to form $M \times M$ $[V_{mn}]$ and, hence, $[H_{mn}]$ matrices in (2.17). Therefore, the integrals (2.23), which may be written as

$$V_{0,n} = 2\mathcal{N}_0^{(\alpha)}\mathcal{N}_n^{(\alpha)} \int_0^\infty V(r) r^\alpha e^{-r} L_n^{(\alpha)}(r)\, dr \tag{3.2}$$

are to be evaluated for $n = 0, 1, \ldots, 2M - 2$, with their respective potentials being considered.

If we recall the integral formula [24]

$$\int_0^\infty x^\beta e^{-sx} L_n^{(\alpha)}(x)\, dx = \frac{\Gamma(\beta + 1)\Gamma(\alpha + n + 1)}{n!\,\Gamma(\alpha + 1)} s^{-\beta - 1} \times {}_2F_1\left(-n, \beta + 1; \alpha + 1; \frac{1}{s}\right), \tag{3.3}$$

then it follows that

$$V_{0,n} = -\frac{2Z}{\alpha} \frac{\mathcal{N}_0^{(\alpha)}}{\mathcal{N}_n^{(\alpha)}} (1 + \gamma)^{-\alpha} \times {}_2F_1\left(-n, \alpha; \alpha + 1; \frac{1}{1 + \gamma}\right) \tag{3.4}$$

for the Yukawa potential in (1.2), where ${}_2F_1(a, b; c; x)$ stands for the Gauss hypergeometric function. Alternatively, it may be seen from (2.13) that

$$V_{0,n} = -2Z\mathcal{N}_0^{(\alpha)}\mathcal{N}_n^{(\alpha)} \sum_{k=0}^{n} \times \int_0^\infty r^{\alpha - 1} e^{-(1+\gamma)r} L_k^{(\alpha-1)}(r)\, dr \tag{3.5}$$

for which the formula (3.3) now implies the expression

$$V_{0,n} = -2Z\mathcal{N}_0^{(\alpha)}\mathcal{N}_n^{(\alpha)}(1 + \gamma)^{-\alpha} \times \sum_{k=0}^{n} \frac{\Gamma(\alpha + k)}{k!} \left(1 - \frac{1}{1 + \gamma}\right)^k, \tag{3.6}$$

where we have used the identity

$${}_2F_1(-k, b; b; x) = (1 - x)^k \tag{3.7}$$

known for the hypergeometric function [25]. As a matter of fact, the hypergeometric series in (3.4) terminates to give a polynomial of degree n in inverse powers of $1 + \gamma$, since its first parameter is equal to a negative integer $-n$. Thus for the Yukawa potential, $V_{0,n}$ is expressible as a finite sum in each case of (3.4) and (3.6), which can easily be evaluated.

A linear transformation on r shows that the Hamiltonian for the Yukawa potential has the scaling properties

$$\begin{aligned} \mathscr{H}(r; Z, \gamma Z) &= Z^2 \mathscr{H}(r; 1, \gamma), \\ E(Z, \gamma Z) &= Z^2 E(1, \gamma), \end{aligned} \tag{3.8}$$

and that the effective parameter in the system is γ, the screening constant. Therefore, setting $Z = 1$ it is enough to determine $E(1, \gamma) \equiv E(\gamma)$. However, the relation in (3.8), $E(\gamma) = E(Z, \gamma Z)/Z^2$, implies the use of the nuclear charge as a flexible convergence parameter in calculating $E(\gamma)$.

The exponential cosine screened Coulomb potential described by (1.3) admits similar scaling relationships

$$\begin{aligned} \mathscr{H}(r; Z, \gamma Z, \lambda Z) &= Z^2 \mathscr{H}(r; 1, \gamma, \lambda), \\ E(Z, \gamma Z, \lambda Z) &= Z^2 E(1, \gamma, \lambda) \end{aligned} \tag{3.9}$$

so that Z may be regarded again as an optimization parameter in the algorithm to determine $E(\gamma, \lambda)$ with two effective coupling constants. On the other hand, in evaluating the matrix elements V_{mn} we take into account the complex-valued integral

$$W_n = I_n(\alpha, \gamma, \lambda) + iJ_n(\alpha, \gamma, \lambda) = \int_0^\infty e^{-(1 + \gamma + i\lambda)r} r^{\alpha - 1} L_n^{(\alpha)}(r)\, dr, \qquad i^2 = -1 \tag{3.10}$$

whose real part I_n,

$$I_n(\alpha, \gamma, \lambda) = \int_0^\infty e^{-(1+\gamma)r} r^{\alpha-1} \cos \lambda r L_n^{(\alpha)}(r)\, dr, \tag{3.11}$$

appears as a factor in $V_{0,n}$ such that

$$V_{0,n} = -2Z\mathcal{N}_0^{(\alpha)}\mathcal{N}_n^{(\alpha)} I_n(\alpha, \gamma, \lambda). \tag{3.12}$$

Making use of (3.3) once more, we find that

$$\alpha n!\, W_n = \Gamma(\alpha + n + 1)(1 + \gamma + i\lambda)^{-\alpha} \times {}_2F_1\left(-n, \alpha; \alpha + 1; \frac{1}{1 + \gamma + i\lambda}\right) \tag{3.13}$$

and that

$$I_n = \frac{(\alpha+1)_n}{n!} \sum_{k=0}^{n} \frac{\Gamma(\alpha + k)(-n)_k}{(\alpha+1)_k k!} \times \left[(1+\gamma)^2 + \lambda^2\right]^{-(1/2)(\alpha+k)} \cos \Theta_k(\alpha, \gamma, \lambda), \tag{3.14}$$

where

$$\Theta_k(\alpha, \gamma, \lambda) = (\alpha + k)\arctan\left(\frac{\lambda}{1+\gamma}\right) \tag{3.15}$$

and the $(a)_k$'s denote the Pochhammer's symbol. Clearly, (3.12) reduces to (3.4) when $\lambda = 0$.

In the numerical Tables (I–V), we present the discrete eigenvalues $E_{n_r,l}$ of the aforementioned

TABLE I

The energy eigenvalues of the screened Coulomb potentials in three dimensions for 1s state, where $n_r = l = 0$, as a function of the parameters γ and λ.[a]

γ	λ	$E_{00}(\gamma, \lambda) = E_{00}(Z, \gamma Z, \lambda Z)/Z^2$	M	Z
0.05	0	−0.451 816 428 524 505 543 856 217	10	0.50
	0.05	−0.450 117 466 420 687 668 045 276	10	0.50
	0.10	−0.445 058 030 645 533 927 672 615	11	0.45
0.10	0	−0.407 058 030 613 403 156 754 507	13	0.50
	0.05	−0.405 507 412 931 225 675 431 785	12	0.50
	0.10	−0.400 884 774 639 478 191 787 512	13	0.45
0.15	0	−0.365 460 799 921 793 890 266 105	15	0.50
	0.05	−0.364 040 916 722 240 150 823 039	14	0.50
	0.10	−0.359 804 685 334 755 576 627 176	15	0.45
0.20	0	−0.326 808 511 369 193 384 882 495	18	0.50
	0.05	−0.325 505 657 332 389 166 011 562	17	0.50
	0.10	−0.321 616 304 846 079 335 403 341	16	0.45
0.30	0	−0.257 638 586 303 054 148 878 964	22	0.50
	0.05	−0.256 538 964 159 520 533 444 154	21	0.50
	0.10	−0.253 253 828 006 553 722 745 643	19	0.45
0.40	0	−0.198 376 083 361 850 216 608 414	26	0.50
	0.05	−0.197 449 760 351 259 487 791 589	23	0.45
	0.10	−0.194 681 361 574 899 112 247 500	23	0.45
0.50	0	−0.148 117 021 889 932 616 711 758	29	0.50
	0.05	−0.147 342 740 117 720 657 806 509	27	0.45
	0.10	−0.145 028 638 481 977 144 542 043	27	0.45
0.75	0	−0.057 400 892 651 401 113 196 797	40	0.50
	0.05	−0.056 946 356 985 538 773 206 001	38	0.50
	0.10	−0.055 590 038 786 699 011 712 910	38	0.50
1.00	0	−0.010 285 798 990 017 696 804 774	72	0.80
	0.05	−0.010 099 990 197 734 283 981 480	70	0.80
	0.10	−0.009 550 829 338 579 678 418 334	70	0.80

[a] The results for which $\lambda = 0$ corresponds to that of the Yukawa potential.

TABLE II

The energy eigenvalues of the screened Coulomb potentials in three dimensions for $2s$ state, where $n_r = 1$ and $l = 0$, as a function of the parameters γ and λ.[a]

γ	λ	$E_{10}(\gamma, \lambda) = E_{10}(Z, \gamma Z, \lambda Z)/Z^2$	M	Z
0.01	0	−0.115 293 285 167 994 256 222 046	10	1.00
	0.05	−0.108 438 269 241 975 709 940 798	17	1.00
	0.10	−0.089 314 822 600 643 154 704 987	20	0.75
0.02	0	−0.106 148 320 244 695 503 250 708	11	1.00
	0.05	−0.099 722 315 288 814 198 046 240	16	1.00
	0.10	−0.081 696 058 253 066 397 242 380	20	0.75
0.03	0	−0.097 531 786 134 660 862 770 039	13	1.00
	0.05	−0.091 501 139 415 524 527 650 863	16	1.00
	0.10	−0.074 505 477 065 191 850 225 935	21	0.85
0.04	0	−0.089 414 634 185 159 188 415 715	15	1.00
	0.05	−0.083 750 777 994 127 510 332 204	16	1.00
	0.10	−0.067 727 101 124 446 391 141 223	21	0.90
0.05	0	−0.081 771 195 795 253 124 173 489	16	1.00
	0.05	−0.076 449 596 250 247 744 384 067	17	1.00
	0.10	−0.061 346 035 868 165 761 960 946	21	0.90
0.10	0	−0.049 928 271 331 918 889 234 997	22	1.00
	0.05	−0.046 046 083 409 608 468 814 342	22	1.00
	0.10	−0.034 941 311 947 228 078 394 017	25	0.95
0.15	0	−0.027 222 190 725 688 518 250 187	28	1.00
	0.05	−0.024 481 216 787 837 974 134 560	28	1.05
	0.10	−0.016 691 259 027 974 294 452 954	31	1.20
0.20	0	−0.012 107 865 195 440 464 385 855	36	1.15
	0.05	−0.010 332 902 275 604 741 148 837	36	1.20
	0.10	−0.005 473 301 991 341 432 457 203	43	1.50
0.25	0	−0.003 395 906 283 239 307 796 442	55	1.55
	0.05	−0.002 484 983 035 290 339 958 215	60	1.65
	0.10	−0.000 426 382 886 554 166 963 351	80	2.60

[a] The results for which $\lambda = 0$ correspond to that of the Yukawa potential.

screened Coulomb potentials as a function of the parameters γ and λ, only for $1s$ ($n_r = l = 0$), $2s$ ($n_r = 1$, $l = 0$), $2p$ ($n_r = 0$, $l = 1$), $3s$ ($n_r = 2$, $l = 0$), and $3p$ ($n_r = l = 1$) states. Further results, which have not been quoted in this article, are available from the author.

4. Further Applications and Discussion

Before discussing the numerical results yielded by the method for the Yukawa and the exponential cosine screened Coulomb potentials, it should be mentioned that some other systems may also be handled in this context. For instance, the wave function for the Schrödinger equation with the Morse potential,

$$V(r) = c[e^{-2a(r-b)} - 2e^{-a(r-b)}], \qquad a, b, c > 0 \tag{4.1}$$

or with the Gaussian potential,

$$V(r) = -ce^{-\mu r^2}, \qquad c, \mu > 0 \tag{4.2}$$

has virtually the same asymptotic form with those of the screened Coulomb potentials, which is reflected successfully by the present Laguerre basis.

The hydrogen-like systems consist of the infinite Coulomb well at $r = 0$, whereas the Morse and the Gaussian potentials are both bounded below with a finite well of depth $-c$ situated at $r = b$ and $r = 0$, respectively. However, this discrepancy is not expected to change the spectral properties to a

TABLE III

The energy eigenvalues of the screened Coulomb potentials in three dimensions for $2p$ state, where $n_r = 0$ and $l = 1$, as a function of the parameters γ and λ.[a]

γ	λ	$E_{01}(\gamma, \lambda) = E_{01}(Z, \gamma Z, \lambda Z)/Z^2$	M	Z
0.010	0	−0.115 245 224 090 564 185 894 783	8	1.00
	0.05	−0.109 466 753 312 547 952 730 780	14	0.95
	0.10	−0.093 254 546 701 988 779 477 545	18	0.75
0.020	0	−0.105 963 398 179 939 904 755 731	10	1.00
	0.05	−0.100 490 560 077 674 317 929 230	14	0.95
	0.10	−0.085 050 687 063 065 300 440 270	18	0.75
0.030	0	−0.097 131 366 795 691 310 671 784	12	1.00
	0.05	−0.091 940 838 774 742 473 748 776	13	0.90
	0.10	−0.077 228 588 374 730 165 798 355	18	0.80
0.040	0	−0.088 729 373 582 879 526 287 939	13	1.00
	0.05	−0.083 801 650 592 422 129 339 538	14	0.90
	0.10	−0.069 778 444 283 779 497 639 945	19	0.85
0.050	0	−0.080 740 387 037 784 609 712 103	14	0.95
	0.05	−0.076 059 012 441 731 047 354 937	14	0.95
	0.10	−0.062 691 517 061 121 333 705 399	19	0.85
0.075	0	−0.062 482 377 022 724 978 944 454	17	0.95
	0.05	−0.058 360 229 161 435 500 909 982	16	1.00
	0.10	−0.046 514 949 552 341 257 460 943	21	0.95
0.100	0	−0.046 534 390 486 724 608 386 601	21	0.95
	0.05	−0.042 912 719 295 762 748 890 806	20	1.00
	0.10	−0.032 468 805 180 794 407 604 986	24	1.00
0.150	0	−0.021 104 888 927 736 242 916 943	27	1.10
	0.05	−0.018 393 378 924 009 668 334 757	27	1.15
	0.10	−0.010 614 296 481 640 512 647 288	32	1.30
0.200	0	−0.004 101 646 530 784 090 388 447	48	1.55
	0.02	−0.003 818 142 955 569 071 678 147	46	1.55
	0.05	−0.002 374 593 515 397 975 627 173	52	1.75

[a] The results for which $\lambda = 0$ correspond to that of the Yukawa potential.

large extent. Actually, all these potentials have a finite number of discrete states located specially on the negative real axis and a continuous spectrum which covers the entire positive real axis in the energy complex plane. Only the exponential cosine screened Coulomb potential may have some discrete energy levels which are positive, depending on the screening constants, γ and λ. Therefore, the present basis set seems to be applicable to the bound state investigations of the potentials in (4.1) and (4.2) as well.

The numerical analysis of the spectra of the Morse and the Gaussian potentials is left to a future study. We have, however, a couple of comments about the determination of their matrix elements. From (3.2), $V_{0,n}$ reads as

$$V_{0,n} = 2c\mathcal{N}_0^{(\alpha)}\mathcal{N}_n^{(\alpha)} \times \int_0^\infty [e^{-2a(r-b)} - 2e^{-a(r-b)}] r^\alpha e^{-r} L_n^{(\alpha)}(r)\, dr \quad (4.3)$$

for the Morse potential, which is evaluated analytically. Indeed, we find, from (3.3) and (3.7), that

$$V_{0,n} = 2ca^n e^{ab} \frac{\mathcal{N}_0^{(\alpha)}}{\mathcal{N}_n^{(\alpha)}} \times [2^n e^{ab}(2a+1)^{-\alpha-n-1} - 2(a+1)^{-\alpha-n-1}] \quad (4.4)$$

TABLE IV

The energy eigenvalues of the screened Coulomb potentials in three dimensions for 3*s* state, where $n_r = 2$ and $l = 0$, as a function of the parameters γ and λ.[a]

γ	λ	$E_{20}(\gamma, \lambda) = E_{20}(Z, \gamma Z, \lambda Z)/Z^2$	M	Z
0.005	0	−0.050 720 178 473 178 174 475 578	10	1.50
	0.01	−0.050 096 692 964 104 121 758 864	12	1.50
	0.05	−0.036 360 827 274 713 626 509 605	20	1.20
0.010	0	−0.046 198 857 799 033 191 519 298	12	1.50
	0.01	−0.045 619 079 544 659 427 108 702	12	1.50
	0.05	−0.032 758 428 702 547 879 110 338	21	1.25
0.015	0	−0.041 971 321 344 717 689 300 636	13	1.45
	0.01	−0.041 431 410 214 832 163 061 802	12	1.50
	0.05	−0.029 387 529 625 298 900 490 129	22	1.25
0.020	0	−0.038 020 014 393 017 364 134 542	15	1.45
	0.01	−0.037 516 772 120 224 993 447 490	14	1.50
	0.05	−0.026 238 981 974 258 006 477 397	22	1.35
0.030	0	−0.030 886 083 779 974 481 232 732	17	1.45
	0.01	−0.030 448 461 956 868 992 219 576	17	1.50
	0.05	−0.020 575 395 836 375 598 616 748	22	1.45
0.040	0	−0.024 692 267 257 683 267 057 858	20	1.45
	0.01	−0.024 312 219 417 009 192 480 301	19	1.50
	0.05	−0.015 705 796 903 475 525 843 015	22	1.55
0.050	0	−0.019 352 554 814 752 342 295 398	23	1.50
	0.01	−0.019 023 937 729 678 813 513 616	22	1.50
	0.05	−0.011 575 564 207 060 795 847 556	26	1.65
0.075	0	−0.009 285 396 101 760 038 390 013	30	1.65
	0.01	−0.009 066 400 261 165 411 682 742	31	1.65
	0.05	−0.004 179 119 076 260 311 098 934	35	2.00
0.100	0	−0.003 208 046 744 690 258 718 214	45	2.00
	0.01	−0.003 081 064 010 465 364 747 867	45	2.00
	0.02	−0.002 708 053 231 650 741 847 762	45	2.10

[a] The results for which $\lambda = 0$ correspond to that of the Yukawa potential.

with $n = 0, 1, \ldots$. However, similar calculations for the Gaussian potential lead to the integrals of the type

$$V_{0,n} = -2c\mathcal{N}_0^{(\alpha)}\mathcal{N}_n^{(\alpha)} \int_0^\infty e^{-\mu r^2 - r} r^\alpha L_n^{(\alpha)}(r)\, dr, \quad (4.5)$$

which cannot be expressed as a finite combination of elementary functions. As a result, numerical integration or other techniques will be necessary for obtaining the zeroth-row entries of the matrix $[V_{mn}]$ in this case of the Gaussian potential.

The low-lying state eigenvalues $1s$, $2s$, $2p$, $3s$, and $3p$ of the screened Coulomb potentials are tabulated to 24 significant decimal points in Tables I–V. In the tables, M denotes the dimension of the subspace spanned by the Laguerre basis, or the truncation order of the wave function. Meanwhile, we include also the effective charge parameters Z for which the best converged results are obtained. The three-dimensional calculations are presented setting the space dimension $N = 3$, so that the eigenvalues are $E^{(3)}_{n_r, l}$ in the notation of Section 1.

It is well known for the Yukawa potential, where $\lambda = 0$, that there exists a threshold value of the screening parameter γ, γ_{thr} say, beyond which the particular bound state being considered cannot survive anymore. It is worth mentioning here the exact threshold values listed in Table VI, which were calculated by Demiralp in [26]. Hence, the range of the parameter γ in our numerical tables has been specified according to Table VI, so as to cover roughly the region in which $0 < \gamma < \gamma_{\text{thr}}$.

TABLE V

The energy eigenvalues of the screened Coulomb potentials in three dimensions for $3p$ state, where $n_r = l = 1$, as a function of the parameters γ and λ.[a]

γ	λ	$E_{11}(\gamma, \lambda) = E_{11}(Z, \gamma Z, \lambda Z) / Z^2$	M	Z
0.005	0	−0.050 708 224 175 839 214 790 596	9	1.50
	0.01	−0.050 128 133 804 460 003 595 342	11	1.50
	0.05	−0.037 319 320 114 986 477 048 010	19	1.20
0.010	0	−0.046 153 104 829 162 287 315 274	11	1.50
	0.01	−0.045 611 041 324 099 095 230 270	11	1.50
	0.05	−0.033 558 447 061 411 274 634 728	19	1.20
0.015	0	−0.041 872 798 771 094 105 666 978	12	1.45
	0.01	−0.041 365 467 297 671 881 713 156	11	1.50
	0.05	−0.030 019 793 704 493 151 733 488	19	1.25
0.020	0	−0.037 852 389 200 223 176 326 568	14	1.45
	0.01	−0.037 377 066 115 630 550 712 958	13	1.50
	0.05	−0.026 696 021 052 723 164 942 072	20	1.30
0.030	0	−0.030 540 967 584 512 981 172 893	16	1.45
	0.01	−0.030 123 168 664 050 780 131 022	16	1.50
	0.05	−0.020 666 880 487 653 454 712 655	20	1.45
0.040	0	−0.024 132 353 610 390 802 462 032	19	1.50
	0.01	−0.023 765 446 338 580 927 971 066	18	1.50
	0.05	−0.015 424 146 289 428 831 669 006	21	1.55
0.050	0	−0.018 557 751 883 405 996 604 894	22	1.50
	0.01	−0.018 236 857 481 007 000 622 255	22	1.55
	0.05	−0.010 929 329 822 556 161 248 565	25	1.65
0.075	0	−0.007 928 707 186 332 842 403 447	30	1.70
	0.01	−0.007 709 405 861 288 180 529 436	30	1.70
	0.05	−0.002 793 773 729 583 978 343 746	35	2.30
0.100	0	−0.001 589 001 525 867 560 267 559	48	2.35
	0.01	−0.001 465 954 382 433 222 130 747	48	2.40
	0.02	−0.001 107 425 004 372 140 674 334	51	2.55

[a] The results for which $\lambda = 0$ correspond to that of the Yukawa potential.

On the other hand, for sufficiently small γ and large enough λ values, the exponential cosine screened Coulomb potential becomes nearly a periodic potential which is subjected to another course. The inspection of the references cited in Section 1 shows that the main interest lies in the case of small λ regime, with $\lambda \approx \gamma$. We, therefore, consider the range $0 \leq \lambda \leq 0.10$ of the second screening parameter in the tables, where the exponential cosine screened Coulomb potential tends to zero with weak oscillations about r axis, as r increases.

TABLE VI

The threshold values of γ in the case of the Yukawa potential, calculated by Demiralp in [21], for the states considered numerically in this work.

State	γ_{thr}
$1s$	1.190 612 421
$2s$	0.310 209 283
$2p$	0.220 216 807
$3s$	0.139 450 294
$3p$	0.112 710 498

The numerical results verify evidently that the present Laguerre basis is particularly efficient for all screening parameters γ, which are not in the near vicinity of γ_{thr}. In fact, most of the methods applied to a problem of this kind, wherein both discrete and continuous spectra appear, fail in finding the eigenvalues at the border of the continuum. We notice that for very weakly bound states, with E just below zero, the truncation order M required to achieve the convergence rises dramati-

cally. Furthermore, numerical experiments showed that the algorithm is very sensitive to numerical error accumulations for relatively large matrix sizes, typically, when $M > 40$. This causes an oscillating character in the last decimal points of the calculated eigenvalues. For this reason, the selection of a suitable parameter Z, which yields a reasonable convergence in M, gains a lot of importance. However, using a multiprecision arithmetic on *Mathematica*, for example, reliable information and hence accurate results can be obtained almost everywhere in the domain of the screening constants for any value of Z.

Consequently, if we cite here a series of our articles on two- and N-dimensional isotropic polynomial oscillators [27, 28], this study may be regarded as a continuation of such strongly convergent variational methods for quantum problems, which deals with nonpolynomial potentials.

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