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Abstract
The Gaussian, exponential and Laguerre basis functions are examined in a variational calculation of energies and wavefunctions. The Laguerre basis set is already orthonormal and complete, but the Gaussian and exponential basis sets are not orthonormal. We used the linear and Coulomb potentials to test these basis functions. Calculations are performed in both position and momentum space. We also present the results with relativistic kinematics in the momentum space calculation. The Gram–Schmidt procedure is used to orthonormalize the Gaussian and exponential basis sets before using them in the calculations. We show that in the case of a pure linear potential, the orthonormal basis constructed from the Gaussian functions performs much better than the exponential and Laguerre basis for the same number of orthogonal functions. For Coulomb-like potentials, the exponential basis performs better than the other two for the same number of basis functions. The advantage of using these simple basis functions is that for the potentials that we examined, one can approach the lower bound of the low-lying states with very few basis functions.

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(Some figures in this article are in colour only in the electronic version)

1. Introduction

Potential models have been an important technique for understanding the mass spectrum of hadrons composed of two (mesons) or three (baryons) constituent quarks [1–4]. The idea is to use a potential that describes both the long-range quark interaction which produces confinement, plus a shorter range potential that describes asymptotic freedom. A function that grows linearly with distance, which is motivated from studies of lattice gage theory [5], is commonly used as a potential model for the long-range confining interaction

[6]. A function inversely proportional to distance, i.e. a Coulomb-like potential, is often used for the short-range quark interaction and is motivated by high-momentum studies of quantum chromodynamics [7]. These potentials can be inserted into the non-relativistic Schrödinger equation or, with appropriate modifications, can be used in three-dimensional psuedo-relativistic wave equations [8–16] or the fully relativistic bound-state Bethe–Salpeter equation [17–19]. Relativistic effects are important because they are needed to describe various phenomenological properties, such as Regge trajectories [20]. Non-relativistic potential models are successful in describing properties of hadrons containing heavy quarks [21–24], whereas relativistic models need to be used for light quark systems [25]. Nevertheless, the basic paradigm of a Coulomb plus linear potential [26–29] has proved to be very successful in describing a host of hadron properties, such as decay rates and spectroscopy [30–35]. These potentials and their associated bound-state equations are also often studied in momentum space due to the ease of treating relativistic effects [36].

The present paper investigates a particular aspect of linear and Coulomb potentials used for both non-relativistic equations and equations with relativistic kinematics in both position and momentum space. In order to solve a bound-state equation using matrix methods, one is often required to expand the wavefunction in terms of a known set of basis functions. The present work examines three common choices for the basis function set and analyses their behavior with common choices for bound-state equations. This could be useful in making more precise calculations of hadron spectra and decay rates.

There are many ways to calculate the energy spectrum of a given Hamiltonian. A common method is to expand the wavefunction in a complete orthonormal basis set. In practice, one cannot use an infinite number of basis functions and one has to settle for a finite subset, and the wavefunction is expanded as a linear combination of a finite set of orthogonal functions. The expansion coefficients can be treated as variational parameters and the calculation becomes a variational problem. Minimizing the energy with respect to these coefficients leads to a matrix eigenvalue equation which must be solved. The lowest eigenvalue is now the upper bound of the ground-state energy. As the number of functions in the expansion increases, the estimate of the ground-state energy becomes better, although it will achieve the true ground-state energy value only when an infinite number of functions is used. In reality, one can never use an infinite number of functions, and the lowest energy eigenvalue might not be as close as one would like to the true ground-state energy. This can be remedied by including one or more parameters in the basis functions themselves. There are certain complete basis sets that are well known [40], and the above method works very well with these basis functions. We will show that one can construct some simple basis function sets which work very well with only a small number of functions. These basis functions do not have to be orthogonal since they can always be orthonormalized. In this paper, we will present the results obtained for linear and Coulomb potentials.

2. Method

In this paper, a variational wavefunction is constructed from a linear combination of basis functions. Each basis function is a function of r and a single variational parameter. The expectation value of the Hamiltonian is found by using this variational wavefunction, and the energy is minimized with respect to the variational parameter.

The Schrödinger equation for the reduced wavefunction $u_{nl}(r)$ is

$$\frac{-\hbar^2}{2\mu}\frac{\mathrm{d}^2}{\mathrm{d}r^2}u_{nl}(r) + V(r)u_{nl}(r) + \frac{\hbar^2}{2\mu}\frac{l(l+1)}{r^2}u_{nl}(r) = Eu_{nl}(r). \tag{1}$$

The variational wavefunction is a superposition of basis functions,

$$u_{nl}(r) = \sum_{j=1}^{N_{\max}} c_j \tilde{g}_j(r, b), \tag{2}$$

where c_j are the coefficients, the set $\{\tilde{g}_j(r, b)\}$ is an orthonormal set of basis functions and b is the variational parameter. Orthogonal functions are denoted with a tilde as in $\tilde{g}$. If the basis functions $\tilde{g}_j$ form a complete orthonormal set, then in the limit that the number of superimposed basis functions approaches infinity, $N_{\max} \to \infty$, the variational wavefunction will approach the true wavefunction of the Schrödinger equation. In this paper, we consider the linear potential and the Coulomb potential, i.e

$$V(r) = \sigma r \qquad V(r) = -C/r, \tag{3}$$

where σ and C are the coupling constants. This type of confining potential and Coulomb-like potentials are frequently used in the studies of meson mass spectra in the context of quark–antiquark bound states [36, 38]. For the purely linear potential, equation (1), with $l = 0$, can be transformed into the Airy differential equation. The energies are related to the roots of the Airy function x_n by

$$E_{n-1} = \left(\frac{\sigma^2\hbar^2}{2\mu}\right)^{\frac{1}{3}} |x_n|. \tag{4}$$

For example, the ground-state energy E_0 is proportional to the first root of the Airy function x_1. When $l \neq 0$, there is no exact expression for the energy. In the case of pure Coulomb-like potential, we will report the results for $l = 0$ with $C = 1$. We scale the equation in such a way that $E_n = -1/n^2$.

In this paper three different sets of basis functions are used. The first one is the Laguerre basis which is a complete orthonormal basis set. The other two sets are based upon the exponential and Gaussian functions defined as

$$g_i^G(r, b) = N_i^G r^{l+1} \mathrm{e}^{-a_i r^2} \tag{5}$$

and

$$g_i^E(r, b) = N_i^E r^{l+1} \mathrm{e}^{-a_i r}, \tag{6}$$

with the normalization constants

$$N_i^G \equiv \sqrt{\frac{2(2a_i)^{\frac{2l+3}{2}}}{\Gamma\left(\frac{2l+3}{2}\right)}}, \tag{7}$$

and

$$N_i^E \equiv \sqrt{\frac{(2a_i)^{2l+3}}{\Gamma(2l+3)}}. \tag{8}$$

The variational parameter is b and $a_i = (N_{\max} b^2)/i^2$ for the Gaussian basis and $a_i = (i/N_{\max} b)$ for the exponential basis, where $i = 1, 2, 3, \ldots$. The Laguerre basis functions are defined as

$$\tilde{g}_i^L(r, b) = \frac{(br)^{l+1}}{b\sqrt{N_i^L}} L_i^{2l+2}(2br)\, \mathrm{e}^{-br}, \tag{9}$$

where $L_\alpha^\beta(x)$ are the Laguerre polynomials and the normalization is given by

$$N_i^L \equiv b^{-3} \left(\frac{1}{2}\right)^{2l+3} \frac{\Gamma(i + 2l + 3)}{i!}. \tag{10}$$

As before, the variational parameter is b and $i = 0, 1, 2, \ldots$ are the indices. Note that the Laguerre basis set is already orthonormal. Other authors [38, 40] have successfully used the Laguerre basis to solve problems that frequently occur in nuclear and particle physics.

Although analytical expressions for the matrix elements of the non-relativistic kinetic energy operator, the linear potential and the Coulomb potential exist for Laguerre basis functions [38], in this paper we are comparing the efficiency of the Gaussian, exponential and Laguerre basis functions in producing the energy spectrum of a given Hamiltonian. Note that the energy spectra are known for a purely linear potential with $l = 0$ and are given by equation (4). We compare the energy spectra obtained from the three different basis sets while using the same number of basis functions for each basis set. Since the exponential and Gaussian basis functions are not orthonormal, we first construct orthonormal sets $\{\tilde{g}_i\}$ by using the Gram–Schmidt procedure.

For the Gaussian and exponential type of basis functions investigated in this paper, it is numerically impossible to orthonormalize more than a certain number of basis functions. For example, consider the set of functions $\{g_i = \exp[-(N_{\max}/i^2)b^2r^2]\}$. Here $N_{\max}$ is the number of functions to be orthonormalized and $i = 1, 2, \ldots, N_{\max}$. Once $N_{\max}$ is large enough, the contribution from this function is negligible except for very small values of r. Therefore increasing the number of functions to $N_{\max} + 1$ does not necessarily enable us to construct $N_{\max} + 1$ number of orthogonal functions. With the Gaussian basis set we cannot construct more than 15 orthonormal functions with double precision arithmetic and for the exponential basis we cannot go beyond 10 functions.

All the basis function sets are orthonormalized as

$$\int_0^\infty \tilde{g}_i(r, b)\tilde{g}_j(r, b)\,\mathrm{d}r = \delta_{ij}. \tag{11}$$

Now expand the reduced wavefunction in equation (1) by using equation (2). After projecting with $\tilde{g}_j(r)$ and integrating, we obtain

$$\sum_{i=1}^{N_{\max}} c_i \int_0^\infty \tilde{g}_j(r) H \tilde{g}_i(r)\,\mathrm{d}r = E c_j. \tag{12}$$

This is a standard eigenvalue problem, and we can find the eigenenergy and the eigenvectors. Once the eigenvector (the values of the c_i) is found, the wavefunction can be constructed from equation (2).

3. Momentum space

As we mentioned in the introduction, relativistic kinematics can be easily implemented in momentum space. In momentum space the Schrödinger equation is an integral equation written as [36]

$$T(p)\Phi(\mathbf{p}) + \int \langle \mathbf{p}|\hat{V}|\mathbf{p}'\rangle \Phi(\mathbf{p}')\,\mathrm{d}\mathbf{p}' = E\Phi(\mathbf{p}), \tag{13}$$

where $T(p) = p^2/2\mu$ for non-relativistic kinematics (μ is the reduced mass) and $T(p) = \sqrt{p^2 + m_1^2} + \sqrt{p^2 + m_2^2}$ for relativistic kinematics. $\langle \mathbf{p}|\hat{V}|\mathbf{p}'\rangle$ is the Fourier transform of the position space potential $V(r)$. The separation of the angular dependence part can be done by taking $\Phi(\mathbf{p}) = \phi_l(p)Y_l^m(\theta, \phi)$, and we obtain a one-dimensional integral equation

$$T(p)\phi_l(p) + \int_0^\infty V_l(p, p')\phi_l(p')p'^2\,\mathrm{d}p' = E\phi_l(p). \tag{14}$$

Here, $V_l(p, p')$ is the lth partial wave component of the momentum space potential $\langle \mathbf{p}'|\hat{V}|\mathbf{p}\rangle$, and it is given as

$$V_l(p, p') = 2\pi \int_{-1}^{+1} \langle \mathbf{p}'|\hat{V}|\mathbf{p}\rangle P_l(x)\,\mathrm{d}x. \tag{15}$$

$P_l(x)$ is the Legendre polynomial of order l and $x = \cos\theta$. Now the wavefunction $\phi_l(p)$ can be expanded in a basis as

$$\phi_l(p) = \sum_{i=1}^{\mathrm{Nmax}} c_i \tilde{f}_i(p), \tag{16}$$

where $\tilde{f}_i(p)$ are the orthonormal basis functions constructed from $f_i(p)$'s, which are the Fourier–Bessel transforms of the function $g_n(r)$ in equations (5), (6) and (9), and they are related by

$$f_i(p) = \sqrt{\frac{2}{\pi}} \int_0^\infty g_i(r) j_l(pr) r^2\,\mathrm{d}r. \tag{17}$$

The Fourier–Bessel transforms $f_i(p)$ are given by

$$f_i^G(p) = \frac{N_i^G p^l\, \mathrm{e}^{-p^2/4a}}{(2a)^{l+3/2}} \tag{18}$$

$$f_i^E(p) = \sqrt{\frac{2}{\pi}} \frac{N_i^E (2a)(2p)^l \Gamma(l+2)}{(a^2+p^2)^{(l+2)}} \tag{19}$$

$$f_i^L(p) = \frac{1}{\sqrt{N}} \frac{(p/b)^l}{[(p/b)^2+1]^{l+2}} P_i^{(l+3/2, l+1/2)}\left(\frac{p^2-b^2}{p^2+b^2}\right). \tag{20}$$

Here, $f_i^G(p)$, $f_i^E(p)$, $f_i^L(p)$ are the Fourier–Bessel transforms of the Gaussian, exponential and Laguerre, respectively. $P_i^{(l+3/2, l+1/2)}$ is the Jacobi polynomial and N_i^G and N_i^E are the normalizations given in (7) and (8), and the normalizaton for the Fourier–Bessel transform of the Laguerre basis is given by [40]

$$N = \frac{b^3}{2(2i+2l+3)} \frac{\Gamma(i+l+5/2)\Gamma(i+l+3/2)}{i!\Gamma(i+2l+3)}. \tag{21}$$

By expanding the wavefunction in equation (14) in terms of the orthonormalized functions $\tilde{f}_i(p)$ and then by multiplying with $\tilde{f}_j(p)p^2$ and integrating, we obtain

$$\sum_{i=1}^{N\mathrm{max}} c_i \left[\int_0^\infty \tilde{f}_j(p) T(p) \tilde{f}_i(p) p^2\,\mathrm{d}p + \int_0^\infty \int_0^\infty V_l(p, p') \tilde{f}_j(p) \tilde{f}_i(p') p'^2 p^2\,\mathrm{d}p'\,\mathrm{d}p \right] = c_j E. \tag{22}$$

This is a standard matrix eigenvalue equation and can be solved by conventional means. In momentum space, the linear potential and Coulomb-like potentials become singular and subtraction methods must be used. In this paper, we have used the subtraction method developed by Maung *et al* [36, 37]. All necessary details to reproduce the results of this paper can be found in this reference.

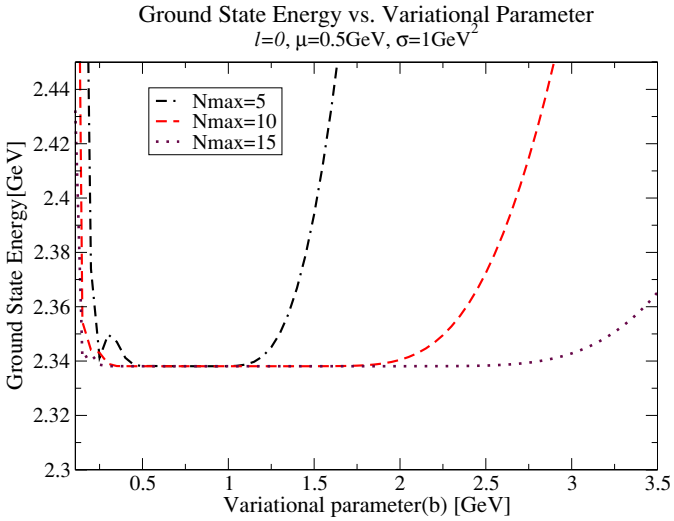

Figure 1. Position space results for the ground-state energy calculated with the Gaussian variational wavefunction are plotted against the variational parameter for $l = 0$. Parameters are $m_1 = m_2 = 1\,\text{GeV}$ and $\sigma = 1\,\text{GeV}^2$. The ground-state energy becomes more independent of the variational parameter when N_{max} is increased.

4. Results

In figure 1 the ground-state energy eigenvalues are plotted with respect to the variational parameter, using the variational wavefunction constructed with the Gaussian basis for a purely linear potential. Units are used in which $\hbar = c = 1$ for all calculations. Also $m_1 = m_2 = 1\,\text{GeV}, \sigma = 1\,\text{GeV}^2$ and $l = 0$. As seen in figure 1, the ground-state energy eigenvalues become less dependent on the variational parameter as the number of basis functions N_{max} increases. The S state energies are given by the roots of the Airy function in equation (4). Table 1 shows that all the energies from 1S to 5S agree with the position space calculations based upon the Gaussian functions with $N_{\text{max}} = 15$. Since all the S state energies are given by the roots of the Airy function, we list the roots in the last column [41]. It can be seen that the exponential function does not perform well compared to the Gaussian function. Table 3 shows the results of the momentum space calculations for the same case and the same conclusion is reached.

For P states, there are no analytical results for a purely linear potential in position space and non-relativistic momentum space. In addition, there are no analytical results for a purely linear potential for S and P states for relativistic momentum space calculations. Therefore, we use the Laguerre basis results with 80 functions as a benchmark for position space, non-relativistic momentum space and relativistic momentum space. Our position space and momentum space calculations agree up to four decimal places for all energies when using 80 Laguerre basis functions. Therefore, we keep only four decimal places for the P states for position space and non-relativistic momentum space. We also keep four decimal places for the S and P states in the relativistic momentum space calculations.

In figure 2, the ground-state energy eigenvalues are plotted as a function of the variational parameter b. Results are shown for the Gaussian, exponential and the Laguerre basis. In each case, the energy eigenvalues become independent of the variational parameter after some

Table 1. Non-relativistic position space results. S state ($l = 0$) energies of the Gaussian, exponential and Laguerre variational wavefunctions for $N_{\max} = 5$, $N_{\max} = 10$ and $N_{\max} = 15$. The last column shows the roots of the Airy function given by Abramowitz and Stegun (A&S) [41]. The results of Laguerre basis with $N_{\max} = 80$ basis functions agree to all digits with A&S. Also, note that the results obtained with 15 Gaussian basis functions agree with A&S to all digits.

Basis function	$N_{\max} = 5$	$N_{\max} = 10$	$N_{\max} = 15$	$N_{\max} = 80$	A&S
Gaussian					
1S	2.338 127 24	2.338 107 41	2.338 107 41		2.338 107 41
2S	4.118 372 80	4.087 949 45	4.087 949 45		4.087 949 44
3S	6.273 183 01	5.520 559 84	5.520 559 83		5.520 559 83
4S	11.376 775 73	6.786 735 66	6.786 708 09		6.786 708 09
5S	30.017 629 06	7.947 670 45	7.944 133 59		7.944 133 59
Exponential					
1S	2.339 283 09	2.338 109 44			2.338 107 41
2S	4.188 958 61	4.088 270 46			4.087 949 44
3S	5.860 557 14	5.524 152 63			5.520 559 83
4S	14.168 584 14	6.832 405 01			6.786 708 09
5S	75.589 991 49	8.340 714 92			7.944 133 59
Laguerre					
1S	2.341 364 32	2.338 115 92	2.338 107 44	2.338 107 41	2.338 107 41
2S	4.133 335 25	4.088 575 63	4.087 952 62	4.087 949 44	4.087 949 44
3S	5.725 347 17	5.532 094 61	5.520 734 61	5.520 559 83	5.520 559 83
4S	8.114 237 80	6.838 594 40	6.789 927 19	6.786 708 09	6.786 708 09
5S	15.519 048 79	8.148 924 61	7.961 366 33	7.944 133 59	7.944 133 59

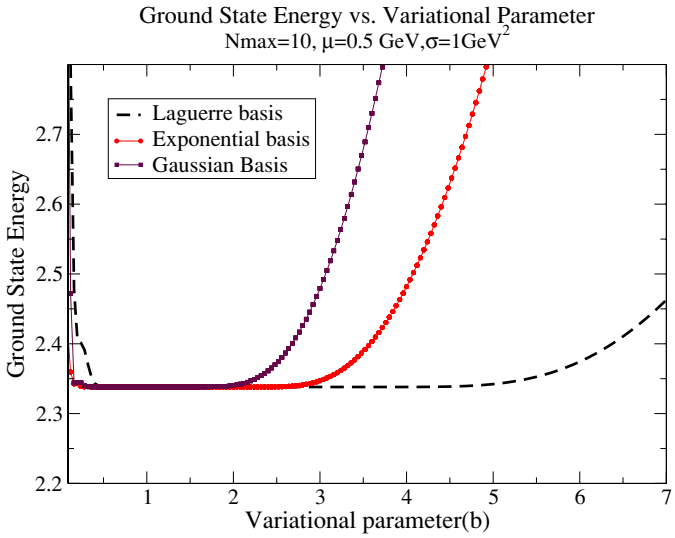

Figure 2. Position space results for the ground-state energy are plotted against the variational parameter for the Gaussian, exponential and Laguerre variational wavefunctions.

initial fluctuations. Note in figure 2 that the energy eventually increases after reaching the minimum. The variational principle requires that the estimated energy approaches an upper bound of the true ground-state energy. Since we use a finite number of basis functions to

Table 2. Non-relativistic position space results. P state ($l = 1$) energies of the Gaussian, exponential and Laguerre variational wavefunctions for $N_{\max} = 5$, $N_{\max} = 10$ and $N_{\max} = 15$. Note that the results of Gaussian basis with $N_{\max} = 15$ agree with the results of Laguerre basis with $N_{\max} = 80$ up to all decimal places. In this table, we keep the results up to four decimal places (see the text).

Basis function	$N_{\max} = 5$	$N_{\max} = 10$	$N_{\max} = 15$	$N_{\max} = 80$
Gaussian				
1P	3.3616	3.3613	3.3613	
2P	4.9692	4.8845	4.8845	
3P	7.3819	6.2076	6.2076	
4P	13.3651	7.4057	7.4057	
5P	36.5071	8.5265	8.5152	
Exponential				
1P	3.3655	3.3613		
2P	5.0092	4.8850		
3P	6.4933	6.2111		
4P	12.7104	7.4956		
5P	51.304	8.8395		
Laguerre				
1P	3.3647	3.3613	3.3613	3.3613
2P	4.9178	4.8856	4.8845	4.8845
3P	6.5930	6.2160	6.2080	6.2076
4P	9.1130	7.4665	7.4083	7.4057
5P	11.5116	8.9001	8.5332	8.5152

construct the variational wavefunction, the energy eventually increases. If it were possible to use an infinite number of basis functions, then the energy would remain constant after reaching the minimum. In table 1, we list the ground-state energy eigenvalues for a purely linear potential with $l = 0$, $m_1 = m_2 = 1$ GeV and $\sigma = 1$ GeV^2. We also list the ground-state energies obtained using the Gaussian, exponential and Laguerre variational wavefunctions. It should be noted that the results with $N_{\max} = 15$ Gaussian basis agree to all decimal places with the exact result [41]. In table 2, the calculations for $l = 1$ are repeated. It is interesting to see that the Gaussian basis performs equally well for this case also. For $l = 1$, there are no analytic results for the energy eigenvalues. Therefore, in the last column, the results from the Laguerre calculations with $N_{\max} = 80$ are listed. This calculation is also verified with momentum space results shown in table 4. We have also done the calculations for $l = 2$ (not listed here) and find that the accuracies obtained for $l = 2$ are comparable with those for $l = 0$ and $l = 1$.

In figure 3, the normalized wavefunctions obtained with $N_{\max} = 1$, 3 and 5 Gaussian basis and $N_{\max} = 80$ Laguerre basis are plotted with respect to the relative distance between the particles. The wavefunction stabilizes as the number of basis functions $N_{\max}$ increases. Note that the wavefunction converges to a common shape when $N_{\max}$ is increased from 3 to 5. Likewise, when $N_{\max}$ is increased further, the shape of the wavefunction remains unchanged. In figure 4, plots are shown for the wavefunctions for the 2S state obtained with $N_{\max} = 2$, 5 and 10 Gaussian basis functions and $N_{\max} = 80$ Laguerre basis functions. The $N_{\max} = 10$ Gaussian results are in agreement with the $N_{\max} = 80$ Laguerre results.

Table 3. Non-relativistic momentum space results; S state ($l = 0$) energies of the Fourier transformed (FT) Gaussian, exponential and Laguerre variational wavefunctions for $N_{\max} = 5$, $N_{\max} = 10$ and $N_{\max} = 15$. The last column shows the roots of the Airy function given by Abramowitz and Stegun (A&S) [41]. Note that the results obtained with 15 Gaussian basis functions agree with A&S to all digits.

Basis function	$N_{\max} = 5$	$N_{\max} = 10$	$N_{\max} = 15$	$N_{\max} = 80$	A&S
FT Gaussian					
1S	2.338 127 24	2.338 107 42	2.338 107 41		2.338 107 41
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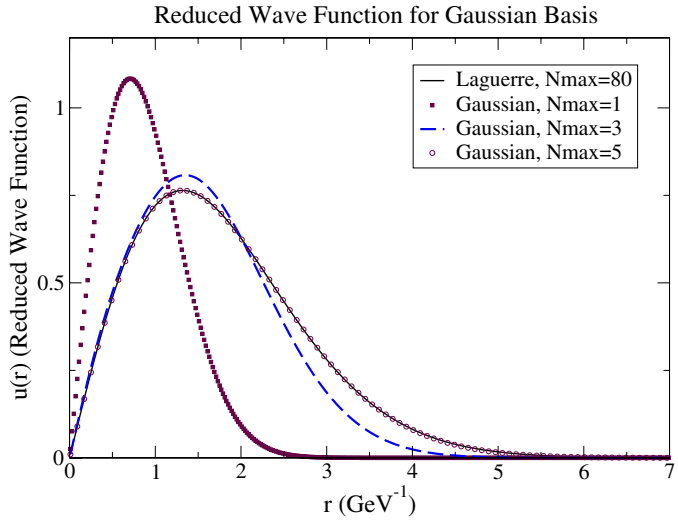

Figure 3. The normalized position space Gaussian variational wavefunctions are plotted for $N_{\max} = 1, 3$ and 5. The wavefunction converges to the Laguerre basis wavefunction constructed from 80 basis functions when $N_{\max}$ is increased from 3 to 5.

Table 4. Non-relativistic momentum space results; P state ($l = 1$) energies of the Fourier transformed (FT) Gaussian, exponential and Laguerre variational wavefunctions for $N_{\max} = 5$, $N_{\max} = 10$ and $N_{\max} = 15$. Note that the results of the Gaussian basis with $N_{\max} = 15$ agree with results of the Laguerre basis with $N_{\max} = 80$ up to all decimal places. In this table we keep the results up to four decimal places (see the text).

Basis function	$N_{\max} = 5$	$N_{\max} = 10$	$N_{\max} = 15$	$N_{\max} = 80$
FT Gaussian				
1P	3.3616	3.3613	3.3613	
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3P	7.3819	6.2076	6.2076	
4P	13.3651	7.4057	7.4057	
5P	36.5071	8.5265	8.5152	
FT exponential				
1P	3.3655	3.3613		
2P	5.0092	4.8850		
3P	6.4933	6.2111		
4P	12.7104	7.4955		
5P	51.3041	8.8395		
FT Laguerre				
1P	3.3647	3.3613	3.3613	3.3613
2P	4.9178	4.8856	4.8845	4.8845
3P	6.5930	6.2160	6.2080	6.2076
4P	9.1130	7.4665	7.4083	7.4057
5P	11.5116	8.9001	8.5332	8.5152

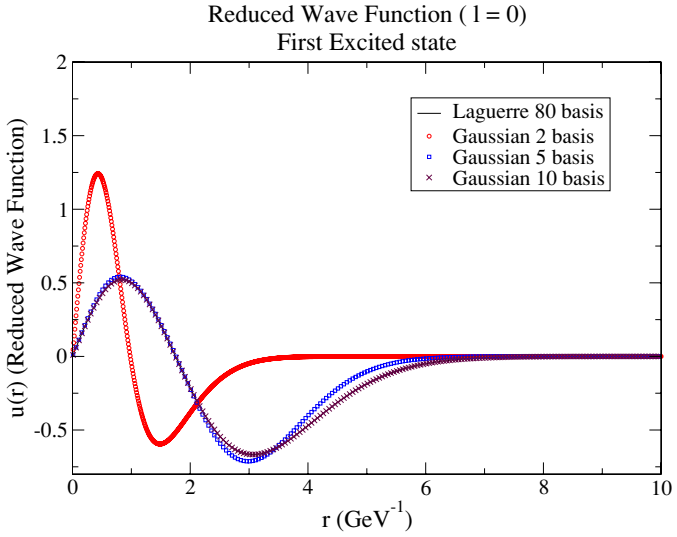

Figure 4. The normalized position space Gaussian variational wavefunctions for the first excited states are plotted for $N_{\max} = 2$, 5 and 10. Note that the wavefunction converges to the Laguerre basis wavefunction constructed from 80 basis functions when $N_{\max}$ is increased from 5 to 10.

Table 5. Relativistic momentum space results; S state ($l = 0$) energies of the Fourier transformed (FT) Gaussian, exponential and Laguerre variational wavefunctions for $N_{\max} = 5$, $N_{\max} = 10$ and $N_{\max} = 15$. Note that the results of the Gaussian basis with $N_{\max} = 15$ agree with results of the Laguerre basis with $N_{\max} = 80$ up to all decimal places. In this table, we keep the results up to four decimal places (see the text).

Basis function	$N_{\max} = 5$	$N_{\max} = 10$	$N_{\max} = 15$	$N_{\max} = 80$
FT Gaussian				
1S	4.1433	4.1433	4.1433	
2S	5.5569	5.5553	5.5553	
3S	6.6732	6.6436	6.6436	
4S	7.9824	7.5645	7.5644	
5S	11.4196	8.3783	8.3782	
FT exponential				
1S	4.1441	4.1433		
2S	5.5631	5.5554		
3S	6.8866	6.6446		
4S	8.3077	7.5737		
5S	16.2128	8.5056		
FT Laguerre				
1S	4.1436	4.1433	4.1433	4.1433
2S	5.5883	5.5556	5.5553	5.5553
3S	7.0207	6.6562	6.6440	6.6436
4S	8.3898	7.6431	7.5689	7.5644
5S	10.4595	8.5748	8.3964	8.3782

It is easier to incorporate relativistic kinematics in momentum space because of the radical $\sqrt{p^2 + m^2}$. One complication in performing calculations in momentum space is that the linear potential and Coulomb-like potentials become singular in momentum space. This can be overcome by using suitable subtraction methods. We perform calculations with relativistic kinematics for the linear potential for $l = 0$ and $l = 1$ and the results are presented in tables 5 and 6. There are no analytical results in the case of relativistic kinematics. Therefore, we calculated the energies with 80 Jacobi (Fourier transform of Laguerre) basis and used them as a benchmark. Again the Gaussian basis performs better than the exponential. We have also done the calculations for $l = 2$ (not listed here) and again find that the accuracies obtained for $l = 2$ are comparable with those for $l = 0$ and $l = 1$.

Next we present the results of the pure Coulomb-like potential for $l = 0$. Table 7 presents the position space calculations, and table 8 presents the momentum space results. For this potential, we scale the Schrödinger equation so that the energy is given by $E_n = -1/n^2$. We see that the exponential basis performs better than the Gaussian and the Laguerre for the same number of basis used. This is not surprising because the ground-state Coulomb wavefunction is proportional to a decaying exponential.

5. Conclusions

In summary, three different basis function sets have been chosen for use in variational calculations. Two are simple basis functions of Gaussian and exponential forms. Before using them in the variational calculations, we construct orthonormal sets. The other one is the Laguerre basis which is orthonormal and complete. For the linear potential, we performed

Table 6. Relativistic momentum space results; P state ($l = 1$) energies of the Fourier transformed (FT) of the Gaussian, exponential and Laguerre variational wavefunctions for $N_{\max} = 5$, $N_{\max} = 10$ and $N_{\max} = 15$. Note that the results of the Gaussian basis with $N_{\max} = 15$ agree with results of the Laguerre basis with $N_{\max} = 80$ up to all decimal places. In this table, we keep the results up to four decimal places (see the text).

Basis function	$N_{\max} = 5$	$N_{\max} = 10$	$N_{\max} = 15$	$N_{\max} = 80$
FT Gaussian				
1P	5.0341	5.0340	5.0340	
2P	6.2012	6.1991	6.1991	
3P	7.2096	7.1702	7.1702	
4P	8.5569	8.0200	8.0200	
5P	12.5293	8.7851	8.7851	
FT exponential				
1P	5.0354	5.0340		
2P	6.2136	6.1992		
3P	7.5188	7.1708		
4P	8.5414	8.0491		
5P	14.0721	8.8737		
FT Laguerre				
1P	5.0375	5.0340	5.0340	5.0340
2P	6.2833	6.2009	6.1991	6.1991
3P	7.4178	7.1853	7.1707	7.1702
4P	8.8923	8.0857	8.0249	8.0200
5P	11.7894	9.2046	8.8465	8.7851

Table 7. Non-relativistic Coulomb position space results. S state ($l = 0$) energies of the Gaussian, exponential and Laguerre variational wavefunctions for $N_{\max} = 5$, $N_{\max} = 10$ and $N_{\max} = 15$. The results of the Laguerre basis with $N_{\max} = 80$ are equal to the values of the scaled Coulomb energy $E = -1/n^2$ and are used as a benchmark.

Basis function	$N_{\max} = 5$	$N_{\max} = 10$	$N_{\max} = 15$	$N_{\max} = 80$ and exact
Gaussian				
1S	−0.99254377	−0.99885192	−0.99936690	
2S		−0.21192874	−0.24693952	
3S			−0.01173145	
4S				
5S				
Exponential				
1S	−1.00000000	−1.00000000		
2S	−0.24975255	−0.25000000		
3S	−0.11099802	−0.11111111		
4S	−0.05749284	−0.06249998		
5S		−0.03962717		
Laguerre				
1S	−1.00000000	−1.00000000	−1.00000000	−1.00000000
2S	−0.24433408	−0.24999824	−0.25000000	−0.25000000
3S		−0.10564871	−0.11102385	−0.11111111
4S			−0.05362321	−0.06250000
5S				−0.04000000

Table 8. Non-relativistic Coulomb momentum space results. S state ($l = 0$) energies of the Fourier transform of the Gaussian, exponential and Laguerre variational wavefunctions for $N_{\max} = 5$, $N_{\max} = 10$ and $N_{\max} = 15$. The results of the Laguerre basis with $N_{\max} = 80$ are equal to the values of the scaled Coulomb energy $E = -1/n^2$ and are used as a benchmark.

Basis function	$N_{\max} = 5$	$N_{\max} = 10$	$N_{\max} = 15$	$N_{\max} = 80$ and exact
FT Gaussian				
1S	−0.99254377	−0.99885192	−0.99936521	
2S		−0.21192874	−0.24693685	
3S			−0.01172791	
4S				
5S				
FT Exponential				
1S	−0.99999995	−0.99999974		
2S	−0.24975237	−0.24999966		
3S	−0.11099779	−0.11111072		
4S	−0.05749251	−0.06249952		
5S		−0.03962332		
FT Laguerre				
1S	−1.00000000	−1.00000000	−1.00000000	−1.00000000
2S	−0.24433408	−0.24999824	−0.25000000	−0.25000000
3S		−0.10564871	−0.11102385	−0.11111111
4S			−0.05362321	−0.06250000
5S				−0.04000000

calculations in both position space and momentum space for $l = 0, 1$ and 2, and for the momentum space calculations we also included relativistic kinematics. For the Coulomb-like potential, we performed the calculations for $l = 0$ in both position space and momentum space. In the case of the linear potential, the results of the Gaussian basis are better than the results of exponential and Laguerre basis for the same number of basis used. This is true for $l = 0$, 1 and 2 and for both non-relativistic and relativistic cases. In the case of the Coulomb-like potential, the exponential basis performs better than the Gaussian and Laguerre basis again for the same number of basis functions used. The disadvantage of using these simple basis functions is that there is an upper limit to the number of orthogonalized functions that can be constructed numerically. But as long as we are interested only in the low-lying states, the use of these simple basis sets is much more efficient.

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