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Useful Bases for Problems in Nuclear and Particle Physics

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A set of exactly computable orthonormal basis functions that are useful in computations involving constituent quarks is presented. These basis functions are distinguished by the property that they fall off algebraically in momentum space and can be exactly Fourier–Bessel transformed. The configuration space functions are associated Laguerre polynomials multiplied by an exponential weight, and their Fourier–Bessel transforms can be expressed in terms of Jacobi polynomials in $\Lambda^2/(k^2 + \Lambda^2)$. A simple model of a meson containing a confined quark-antiquark pair shows that this basis is much better at describing the high-momentum properties of the wave function than the harmonic-oscillator basis.

I. INTRODUCTION

The harmonic oscillator basis has been used extensively in numerical calculations involving confined constituent quarks [1]. The advantage of this basis is that the basis functions are easily computed and Fourier–Bessel transformed. This permits the computation of matrix elements in either a coordinate or momentum representation. For problems involving light quarks, where confined quarks must be treated relativistically, matrix elements of kinetic energy operators that involve square roots, and matrix elements that involve momentum dependent Wigner and/or Melosh rotations are best computed in momentum space. Matrix elements of confining interactions, which are simple to compute in configuration space, require the evaluation of integrals over singular distributions [2] in momentum space. The advantage of the harmonic oscillator basis is that it is straightforward to evaluate both types of matrix elements, completely avoiding difficult calculations.

Although in principle it is possible to perform very accurate model calculations using a harmonic oscillator basis, in practice the oscillator basis does not provide an efficient representation of meson eigenfunctions of mass operators that arise from a linear confinement plus one-gluon-exchange interaction. The reason for this is that the Coulomb part of the one-gluon-exchange interaction leads to momentum-space wave functions that fall off algebraically rather than like Gaussians. This algebraic falloff is also consistent with predictions of asymptotic QCD.

The purpose of this paper is to suggest the use of basis functions that have all of the advantages of the oscillator basis with the additional property that they fall off algebraically in momentum space.

The configuration–space basis functions, sometimes called "Sturmians" [3], have been used successfully in atomic and chemical physics [4, 5] calculations. In this paper, we exploit the fact that they have analytic Fourier–Bessel transforms, and these transforms fall off like polynomials in momentum space. This makes them well suited for models where it is advantageous to work in both configuration and momentum space.

The method is applied to low lying states of a constituent quark model of a meson. The model has a relativistic kinetic energy, a Coulomb interaction, a linear confining interaction, and a smeared out spin–spin interaction. Calculations of eigenfunctions and eigenvalues of this constituent quark mass operator, obtained by projecting the mass operator on the subspace of the Hilbert space spanned by a finite number of these basis states, give converged eigenfunctions and good variational bounds on the mass eigenvalues. In particular, the high-momentum tail of the wave function is described quite well in a truncated basis.

We also discuss briefly the extension of the method to cases where the configuration–space wave function has an integrable fractional power singularity at the origin [6, 7].

II. ELEMENTARY CONSIDERATIONS

In configuration space the radial basis functions are given in terms of polynomials in r times an exponential. An orthonormal basis set is then given by [3]

$$\phi_{nl}(r) = \frac{1}{\sqrt{N_{nl}}} x^l L_n^{(2l+2)}(2x) e^{-x}, \tag{1}$$

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where $x = \Lambda r$, $L_n^{(2l+2)}(x)$ is the associated Laguerre polynomial

$$L_n^{(\alpha)}(x) = \sum_{m=0}^{n} (-)^m \binom{n+\alpha}{n-m} \frac{x^m}{m!} \tag{2}$$

with $\alpha = 2l + 2$ and

$$N_{nl} = \Lambda^{-3} \left(\tfrac{1}{2}\right)^{2l+3} \frac{\Gamma(n+\alpha+1)}{n!} \tag{3}$$

is defined so that the $\phi_{nl}(r)$ satisfy the orthonormality condition

$$\delta_{nm} = \int_0^\infty r^2\, dr\, \phi_n^l(r) \phi_m^l(r). \tag{4}$$

The momentum space functions are the Fourier–Bessel transforms of the $\phi_{nl}(r)$'s,

$$\tilde{\phi}_{nl}(k) = \sqrt{\frac{2}{\pi}} \int_0^\infty r^2\, dr\, j_l(kr) \phi_{nl}(r). \tag{5}$$

They satisfy the orthonormality condition

$$\delta_{nm} = \int_0^\infty k^2\, dk\, \tilde{\phi}_n^l(k) \tilde{\phi}_m^l(k). \tag{6}$$

With these definitions both $\phi_{nl}(r)$ and $\tilde{\phi}_{nl}(k)$ are real.

These functions, along with spherical harmonics, can be used to expand either the momentum or coordinate representations of approximate eigenstates. The coefficients in the expansions

$$\psi(\mathbf{r}) = \sum_{nlm} c_{nlm} \phi_{nl}(r) Y_{lm}(\hat{r}) \tag{7}$$

and

$$\tilde{\psi}(\mathbf{k}) = \sum_{nlm} \tilde{c}_{nlm} \tilde{\phi}_{nl}(k) Y_{lm}(\hat{k}) \tag{8}$$

are related by

$$\tilde{c}_{nlm} = (-i)^l c_{nlm}. \tag{9}$$

These relations follow directly from the formula for the spherical expansions of plane waves [8]. The phase factor ensures that $\tilde{\psi}^*(\mathbf{k}) = \tilde{\psi}(-\mathbf{k})$ for real $\psi(\mathbf{r})$.

We now consider the momentum-space wave function, given by the Fourier–Bessel transform of (1),

$$\tilde{\phi}_{nl}(k) = \sqrt{\frac{2}{\pi}} \int_0^\infty r^2 j_l(kr) \phi_{nl}(r)\, dr. \tag{10}$$

First, we note that the Fourier–Bessel transform of the unnormalized function $r^l e^{-\Lambda r}$ is [9]

$$\sqrt{\frac{2}{\pi}} \int_0^\infty j_l(kr) r^l e^{-\Lambda r} r^2\, dr = \sqrt{\frac{2}{\pi}} \frac{2\Lambda (2k)^l (l+1)!}{(\Lambda^2 + k^2)^{l+2}}. \tag{11}$$

Second, we note that multiplication of the unnormalized function $r^l e^{-\Lambda r}$ by r is equivalent to the operation $-\partial/\partial\Lambda$ on its Fourier–Bessel transform,

$$\sqrt{\frac{2}{\pi}} \int_0^\infty r^2 j_l(kr) r^{l+1} e^{-\Lambda r} = -\frac{\partial}{\partial \Lambda} \left(\sqrt{\frac{2}{\pi}} \frac{(2\Lambda)(2k)^l (l+1)!}{(\Lambda^2 + k^2)^{l+2}} \right). \tag{12}$$

Applying $-\partial/\partial\Lambda$ to the right-hand side of Eq. (12) n times gives the original function multiplied by a polynomial of degree n in $\tau = 1/(k^2 + \Lambda^2)$. In addition the coefficient of the leading power of τ is of the same sign as the coefficient of the leading power of r in the associated Laguerre polynomial. The Fourier–Bessel transform, being unitary, preserves orthonormality. Thus the Fourier–Bessel transform of ϕ_{nl} has the form

$$\tilde{\phi}_{nl}(k) = \frac{k^l}{(\Lambda^2 + k^2)^{l+2}} \times Q_n(\tau), \tag{13}$$

where the $Q_n(\tau)$ are orthogonal polynomials in τ with weight $k^{2l+2}/(\Lambda^2 + k^2)^{2l+4}$. To identify Eq. (13) with the Fourier–Bessel transformation of Eq. (1) it is enough to choose the phase of the normalization constant so the coefficient of τ^n in $Q_n(\tau)$ has the same sign as the coefficient of r^n in $L_n^{2+l}(r)$.

Specifically, one can write

$$\tilde{\phi}_{nl}(k) = \frac{1}{\sqrt{\tilde{N}_{nl}}} \frac{y^l}{(y^2+1)^{l+2}} K_n(u), \tag{14}$$

where $y = k/\Lambda$ and $K_n(u)$ is a polynomial in $u = 1/(y^2 + 1)$ which satisfies the following orthonormality condition,

$$\delta_{nm} = \int_0^\infty k^2\, dk\, \tilde{\phi}_{nl}(k) \tilde{\phi}_{ml}(k). \tag{15}$$

The integral in Eq. (15) can be transformed by the variable change [10],

$$y = \sqrt{\frac{1+x}{1-x}}; \quad dy = \frac{dx}{(1-x)^{3/2}(1+x)^{1/2}}; \quad u = \frac{1-x}{2}, \tag{16}$$

to the integral

$$\delta_{nm} = 2^{-2l-4} \frac{\Lambda^3}{\tilde{N}_{nl}} \int_{-1}^{1} dx (1-x)^{l+3/2} (1+x)^{l+1/2} K_n(u) K_m(u). \tag{17}$$

The polynomials $K_n(u)$ can be expressed in terms of Jacobi polynomials,

$$K_n\left(\frac{1-x}{2}\right) = P_n^{(l+3/2,l+1/2)}(x), \tag{18}$$

where

$$P_n^{\alpha,\beta}(x) = \frac{\Gamma(\alpha+n+1)}{n!\Gamma(\alpha+\beta+n+1)} \sum_{m=0}^{n} \binom{n}{m} \frac{\Gamma(\alpha+\beta+n+m+1)}{2^m\Gamma(\alpha+m+1)} (x-1)^m. \tag{19}$$

This gives the expression for $\tilde{\phi}_{nl}(k)$,

$$\tilde{\phi}_{nl}(k) = \frac{1}{\sqrt{\tilde{N}_{nl}}} \frac{(k/\Lambda)^l}{[(k/\Lambda)^2+1]^{l+2}} P_n^{(l+3/2,l+1/2)}\left[\frac{k^2-\Lambda^2}{k^2+\Lambda^2}\right], \tag{20}$$

where the normalization constant $\tilde{N}_{nl}$ is

$$\tilde{N}_{nl} = \frac{\Lambda^3}{2(2n+2l+3)} \frac{\Gamma(n+l+\frac{5}{2})\Gamma(n+l+\frac{3}{2})}{n!\Gamma(n+2l+3)}. \tag{21}$$

At this point the normalization is determined up to an overall phase. The phase is fixed by requiring the sign of the leading power of r in the associated Laguerre polynomial be the same as the sign of the leading power of $1/(\Lambda^2+k^2)$ appearing in the Jacobi polynomial. Inspection of Eqs. (2), (19), and (20) show that the phases are $(-)^n$ in both cases. This shows that (20) is the Fourier–Bessel transform of (1).

III. APPLICATION

To test the method, we consider a model [11] of a meson consisting of a bound quark–antiquark pair. The mass operator (Hamiltonian in the center-of-momentum frame) is

$$M = 2\sqrt{\mathbf{k}^2+m^2} - \frac{\alpha_s}{r} + \beta r + \gamma + \alpha_s e^{-r^2/4r_0^2} \frac{2s(s+1)-3}{12m^2 r_0^3\sqrt{\pi}}. \tag{22}$$

TABLE I

Eigenvalues of the Pion Mass Operator Using the Polynomial Basis

Basis	M
10	0.14071
20	0.14037
40	0.14019
80	0.14013

The parameter values $\alpha_s = 0.5$, $\beta = 0.197$ GeV^2, $\gamma = -0.777$ GeV, quark mass $m = 0.36$ GeV, and $r_0 = 0.66$ GeV^{-1}. The parameters γ and ρ are chosen to provide a fit to the physical π and ρ masses of 0.140 GeV and 0.784 GeV, respectively.

The mass operator is diagonalized using 10, 20, 40, and 80 basis states. The momentum scale $\Lambda = 2.0$ GeV is chosen to minimize the mass eigenvalue for 10 basis states. The eigenvalues are given in Table I. The corresponding momentum wave functions are shown in Fig. 1. Using only 10 basis states, the wave function is quite stable up to $k = 15$ GeV.

The calculations are done using recursion relations to compute both the associated Laguerre and Jacobi polynomials:

$$(n+1)L_{n+1}^{(\alpha)}(x) = (2n+\alpha+1-x)L_n^{(\alpha)}(x) - (n+\alpha)L_{n-1}^{(\alpha)}(x), \tag{23}$$

and

$$\begin{aligned} 2(n+1)(n+\alpha+\beta+1)(2n+\alpha+\beta)P_{n+1}^{(\alpha,\beta)}(x) \\ = [(2n+\alpha+\beta+1)(\alpha^2-\beta^2) \\ (2n+\alpha+\beta)(2n+\alpha+\beta+1)(2n+\alpha+\beta+2)x]P_n^{(\alpha,\beta)}(x) \\ - 2(n+\alpha)(n+\beta)(2n+\alpha+\beta+2)P_{n-1}^{(\alpha,\beta)}(x). \end{aligned} \tag{24}$$

For comparison purposes, we have also solved the eigenvalue problem with a harmonic oscillator basis, with

$$\tilde{\phi}_{nl}(k) = \frac{1}{\sqrt{\tilde{N}}} y^l L_n^{(l+1/2)}(y^2) e^{-y^2/2}. \tag{25}$$

The mass operator is again diagonalized using 10, 20, 40, and 80 basis states. The momentum scale $\Lambda = 0.9$ GeV is chosen to minimize the mass eigenvalue for 10 basis states. The eigenvalues are given in Table II. Convergence to the exact eigenvalue is much slower than with the polynomial basis. The corresponding momentum wave functions are shown in Fig. 2. For each basis size, the momentum wave

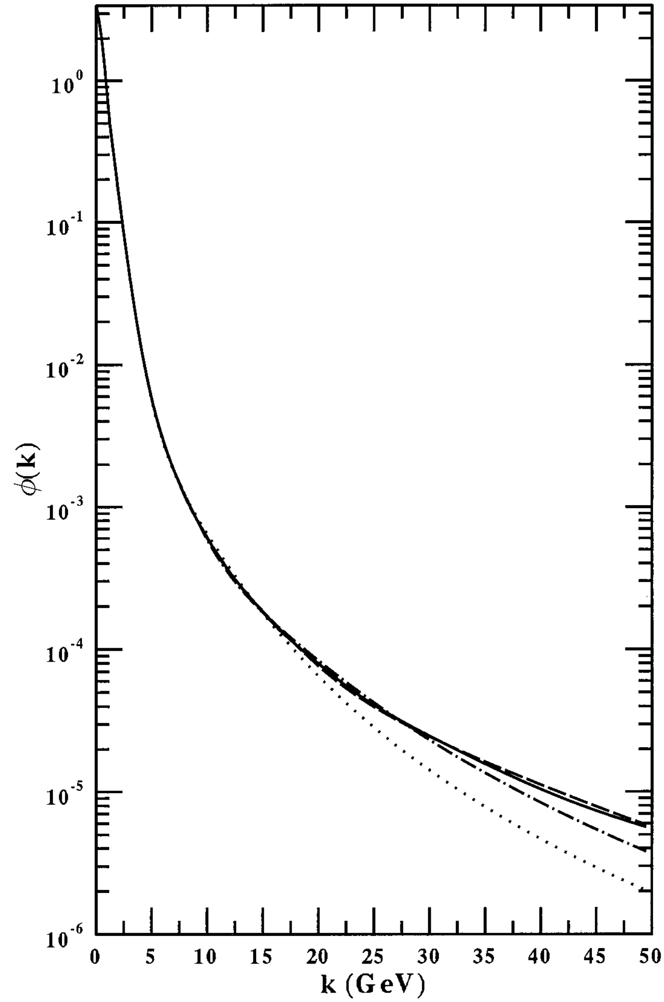

FIG. 1. Pion momentum wave function using the polynomial basis. The dotted, dot-dashed, dashed and solid curves correspond to using 10, 20, 40, and 80 basis functions, respectively.

function is stable until a critical momentum is reached, after which it exhibits a Gaussian falloff characteristic of a truncated oscillator basis. For 10 basis states, this cutoff is about 5 GeV, which may be adequate for use in calculations involving moderate momentum scales (say, 1 GeV, or less), but much better wave functions can be obtained with the same computational investment using the polynomial basis.

TABLE II

Eigenvalues of the Pion Mass Operator using the Oscillator Basis

Basis	M
10	0.14826
20	0.14361
40	0.14186
80	0.14109

IV. INTEGRABLE SINGULARITY

The exact $l = 0$ configuration–space wave function for the model mass operator of Eq. (20) has an integrable singularity [6, 7],

$$\psi(r) \sim \frac{c}{r^{\alpha}} \tag{26}$$

as $r \to 0$. This singularity is seen in numerical calculations based on B-splines in [12] and persists in the presence of the confining interaction.

Naive application of this wave function can lead to unphysical predictions in calculations, such as decay widths, which depend on the value of the wave function at the

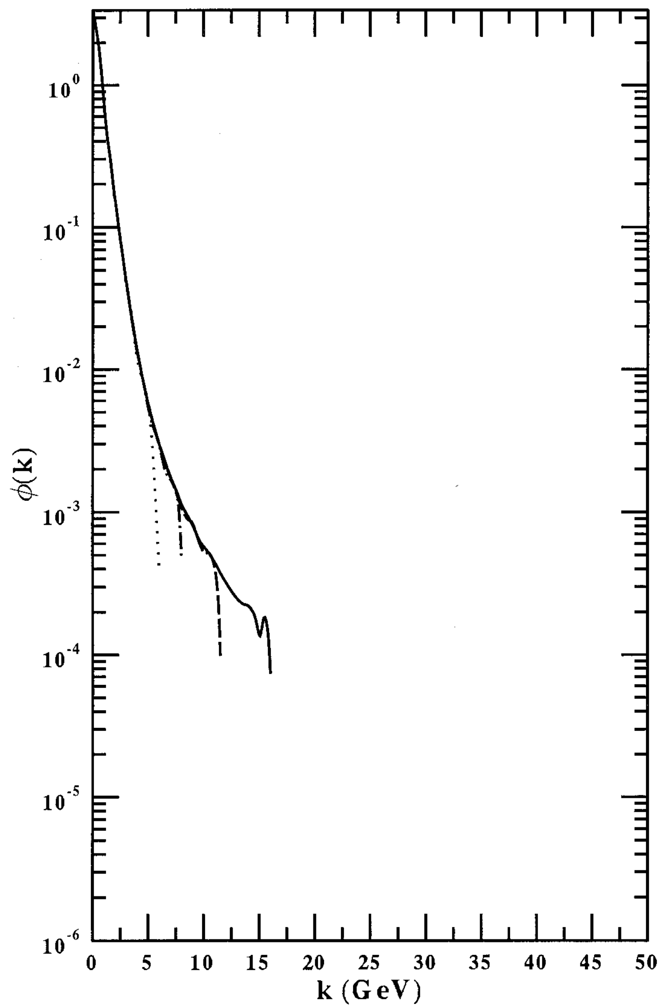

FIG. 2. Pion momentum wave function using the oscillator basis. The dotted, dot-dashed, dashed and solid curves correspond to using 10, 20, 40, and 80 basis functions, respectively.

origin. This is a limitation of this naive model which must be cured by ‘‘correcting’’ the form of the mass operator. Independent of these considerations, it is possible to generalize the methods of this paper to include this mild singularity in the basis functions.

The relevant configuration space basis functions (for $l = 0$) are

$$\phi_n(r) = \frac{1}{\sqrt{N_n}} \frac{e^{-\Lambda r}}{r^{\alpha}} L_n^{2(1-\alpha)}(2\Lambda r) \tag{27}$$

with

$$N_n = \frac{\Gamma(3 - 2\alpha + n)}{n!(2\Lambda)^{3-2\alpha}}. \tag{28}$$

The Fourier–Bessel transforms can be computed explicitly by observing that the Fourier–Bessel transform of

$$\xi_n(r) := r^{n-\alpha} e^{-\Lambda r} \tag{29}$$

is

$$\begin{aligned}\tilde{\xi}_n(k) = {} & \sqrt{\frac{2}{\pi}} \frac{1}{k} \frac{\Gamma(n + 2 - \alpha)}{(\Lambda^2 + k^2)^{(n+2-\alpha)/2}} \\ & \times \sin\left[(n + 2 - \alpha)\tan^{-1}\left(\frac{k}{\Lambda}\right)\right],\end{aligned} \tag{30}$$

which follows from the expressions [13]

$$\int_0^{\infty} e^{-\Lambda r} r^{\mu} J_{\nu}(kr) = \Gamma(\mu + \nu + 1) r^{-(\mu+1)} P_{\mu}^{-\nu}(\Lambda/\sqrt{k^2 + \Lambda^2}) \tag{31}$$

and [14]

$$P_{\mu}^{-1/2}(\cos(\theta)) = \sqrt{\frac{2}{\pi}} \frac{\sin((\nu + 1/2)\theta)}{(\mu + 1/2)\sqrt{\sin(\theta)}}. \tag{32}$$

It follows that

$$\begin{aligned}\tilde{\phi}_n(k) = {} & \frac{1}{\sqrt{N_n}} \sqrt{\frac{2}{\pi}} \sum_{m=0}^{n} (-)^m \binom{n + 2 - 2\alpha}{n - m} \frac{(2\Lambda)^m}{m!} \\ & \times \frac{\Gamma(m + 2 - \alpha)}{(\Lambda^2 + k^2)^{(m+2-\alpha)/2}} \frac{\sin[(m + 2 - \alpha)\tan^{-1}(k/\Lambda)]}{k}.\end{aligned} \tag{33}$$

The relevant basis functions and their Fourier–Bessel transforms can also be computed for $l \neq 0$ using the same methods, but these solutions are not singular at the origin for $l > 0$.

V. CONCLUSION

We have presented a set of exactly computable orthonormal basis functions that are useful in computation involving constituent quarks. The basis functions can be computed easily in both position and momentum space, making it simple to calculate matrix elements in either space. A simple meson model shows that this basis is much better at describing the high-momentum properties of hadronic wave functions than the usual harmonic-oscillator basis, even when only a few configurations are used. The utility of this basis is not diminished in the presence of a spin–spin interaction of a scale to produce the physical π-ρ mass splitting.

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