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Nonperturbative Method for Treating Square Root Operators in Relativistic Quantum Theories

W. N. POLYZOU

Department of Physics and Astronomy,
The University of Iowa,
Iowa City, Iowa 52242

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Numerical methods are developed for computing the discrete spectrum associated with a square root kinetic energy operator. These types of equations are encountered in relativistic quantum mechanical models. We reformulate the dynamical equation into an equivalent equation involving bounded operators. We strongly approximate these operators using matrix elements of operators that do not involve square roots. The method works in both momentum and configuration space. We test the method for a strong Coulomb interaction and for a quark–antiquark potential. We discuss relativistic corrections to the kinetic energy for systems of light quarks. © 1987 Academic Press, Inc.

1. INTRODUCTION

The square root equation,

$$[(-\nabla^2 + m^2)^{1/2} + V]\,\psi = \mu\psi \tag{1.1}$$

was one of the first relativistic generalizations of the Schrödinger equation. It was discarded because of difficulties with the square root operator [1]. In this paper a nonperturbative method for treating the square root operator is presented.

Equations of the form (1.1) occur naturally in Poincaré invariant quantum mechanical models. Poincaré invariance is equivalent to the existence of a continuous unitary representation, $U(A, \alpha)$, of inhomogeneous $SL(2, \mathbb{C})$ on the quantum mechanical Hilbert space [2]. The infinitesimal generators of $U(A, \alpha)$ are the ten self-adjoint operators $\mathbf{H}$, $\vec{\mathbf{P}}$, $\vec{\mathbf{J}}$, $\vec{\mathbf{K}}$. These operators generate time translations, space translations, rotations, and rotationless Lorentz transformations. Physically $\mathbf{H}$, $\vec{\mathbf{P}}$, and $\vec{\mathbf{J}}$ are the Hamiltonian, linear momentum, and angular momentum operators, respectively. The mass operator for this model is

$$\mathbf{M} = {}_+(\mathbf{H}^2 - \vec{\mathbf{P}}\cdot\vec{\mathbf{P}})^{1/2} \tag{1.2}$$

The mass operator $\mathbf{M}$ can be expressed as a noninteracting part, $\mathbf{M}_0$, and an interaction

$$\mathbf{V} := \mathbf{M} - \mathbf{M}_0. \tag{1.3}$$

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The noninteracting part, $\mathbf{M}_0$, is obtained by turning off the interactions in $\mathbf{M}$. The interaction can be anything, although if $\mathbf{M}_0$ describes asymptotic particles, then $\mathbf{V}$ will be short ranged. For two free scalar particles of mass m, the operator $\mathbf{M}_0$ has the form

$$\mathbf{M}_0 = 2(\hat{\mathbf{q}}^2 + m^2)^{1/2}, \tag{1.4}$$

where $\hat{q}$ represents the relative momentum of one of the particles. Equations (1.3) and (1.4) imply the eigenvalue problem

$$[2(\hat{\mathbf{q}}^2 + m^2)^{1/2} + \mathbf{V}]\,\psi = \mu\psi \tag{1.5}$$

for the mass eigenvalue μ. This equation has the same form as Eq. (1.1).

Square root operators also appear in a variety of other related contexts in relativistic quantum mechanics. Examples are:

(1) In the expressions for the many-body forces that are required to maintain cluster separability in the relativistic few-body problem [3].

(2) In the equations that implement the constraints of Poincaré invariance on hadronic current operators [4].

(3) In the expressions for effective relativistic interactions that are obtained from nonrelativistic nucleon–nucleon interactions [5].

(4) In models of confined light quarks [6, 7].

These considerations point to a need for developing numerical methods for treating the square root of an unbounded operator. In this paper methods are developed for constructing eigenfunctions and eigenvalues of (1.1) when μ is in the discrete spectrum of M. The potentials of primary physical interest are the Coulomb potential, the linear potential, and Yukawa-like nuclear potentials.

The main result is that if a basis satisfies certain conditions, then the problem can be solved by matrix algebra. These conditions are given in Section 2. The square roots are treated as square roots of positive symmetric matrices.

The contents of this paper are summarized below. In the next section Eq. (1.1) is reformulated. Finite rank approximate equations are constructed . These equations are the practical basis for the numerical calculations that follow in Section 6. In the third section it is shown that the operators in the approximate equation converge strongly to those of the exact equation when $\mathbf{V}$ is bounded. This condition implies that sequences of approximate eigenvalues converge to exact eigenvalues associated with the discrete spectrum. In Section 4 it is shown that for bases that are easily Fourier transformed, the equations of Section 2 can be modified so that the approximate eigenvalues are variational bounds for the exact ones and the approximate eigenfunctions converge strongly to the exact ones. This method was applied in Ref. [7]. In Section 5 the Culomb, Yukawa, and confining potentials are discussed. In all of these cases $\mathbf{V}$ is not bounded. In Section 6 numerical tests are provided that utilize a spline basis in configuration space. These calculations are

compared to the calculations of Ref. [6] and to variational bounds computed following Section 4. We apply these methods to the problem of examining the size of relativistic corrections to the kinetic energy for systems of light quarks.

2. Finite Rank Approximations

The goal of this paper is to solve the eigenvalue problem

$$\mathbf{M}\psi = \lambda\psi \tag{2.1}$$

numerically on $L^2(\mathbb{R}^3)$, where

$$\mathbf{M} = \mathbf{M}_0 + \mathbf{V} \geqslant 0 \tag{2.2}$$

$$\mathbf{M}_0 = 2(-\nabla^2 + m^2)^{1/2} \tag{2.3}$$

$$\mathbf{V} = \mathbf{V}^\dagger, \qquad |||\mathbf{V}||| < \infty. \tag{2.4}$$

In the above and all that follows, operators are represented by upper case boldface letters. $\|\ \|$ is the norm on $L^2(\mathbb{R}^3)$, and $|||\ |||$ is the norm on $L[L^2(\mathbb{R}^3), L^2(\mathbb{R}^3)]$.

Equation (2.1) is solved by first reformulating the equation so that it becomes a generalized eigenvalue problem formulated with bounded operators. Finite rank approximations of the resulting equation are then made. To perform the first step, multiply both sides of Eq. (2.1) by $\mathbf{M}_0^{-1}$ and factor an $\mathbf{M}_0^{-1}$ out of ψ. This yields the generalized eigenvalue problem

$$(\mathbf{M}_0^{-1} + \mathbf{M}_0^{-1}\mathbf{V}\mathbf{M}_0^{-1})\,\chi = \lambda\mathbf{M}_0^{-2}\,\chi \tag{2.5}$$

$$\psi = \mathbf{M}_0^{-1}\chi. \tag{2.6}$$

The operators in (2.5) and (2.6) have the bounds

$$|||\mathbf{M}_0^{-1}||| = \frac{1}{2m} \tag{2.7}$$

$$|||\mathbf{M}_0^{-2}||| = \frac{1}{4m^2}. \tag{2.8}$$

It follows that

$$|||(\mathbf{M}_0^{-1} + \mathbf{M}_0^{-1}\mathbf{V}\mathbf{M}_0^{-1})||| \leqslant \frac{1}{2m}\left(1 + \frac{|||\mathbf{V}|||}{2m}\right). \tag{2.9}$$

Next, the class of finite dimensional subspaces on which approximate solutions are constructed is defined. Let $\{\mathbf{P}^N\}_{N=1}^{\infty}$ be a collection of finite dimensional orthogonal projection operators with the properties

(P1) $\mathrm{Dim}[\mathrm{Range}(\mathbf{P}^N)] = N$,

(P2) $\mathbf{P}^N\mathbf{P}^{N+K} = \mathbf{P}^N$,

(P3) $s\text{-}\lim_{N\to\infty} \mathbf{P}^N = \mathbf{I}$,

(P4) $\text{Range}(\mathbf{P}^N) \subset \text{Domain}(\mathbf{M}_0^2)$,

(P5) $s\text{-}\lim_{N\to\infty} \mathbf{M}_0^2 \mathbf{P}^N \mathbf{M}_0^{-2} = \mathbf{I}$.

Property (P5) is the only nontrivial restriction on this choice of $\mathbf{P}^N$.

A sufficent condition for property (P5) to hold is that there exists bounded operators $\mathbf{B}_1$ and $\mathbf{B}_2$ such that

(P5′) $\|\!|\, \mathbf{M}_0^2(\mathbf{P}^N - 1)\, \mathbf{M}_0^{-2} \,|\!\| \leqslant \|\!|\, \mathbf{B}^1(\mathbf{P}^N - 1)\, \mathbf{B}_2 \,|\!\|$.

This condition is satisfied by many choices of $\{\mathbf{P}^N\}_{N=1}^{\infty}$.

Instead of specifying a sequence of projection operators, $\{\mathbf{P}^N\}_{N=1}^{\infty}$, satisfying (P1)–(P5), it is sometimes useful to specify a basis $\{\phi_n\}_{n=1}^{\infty}$ that has the property that the first N basis functions span the range of $\mathbf{P}^N$, where the collection $\{\mathbf{P}^N\}_{N=1}^{\infty}$ satisfy (P1)–(P5). Such a basis is called an *acceptable basis*. A basis consisting of momentum space spline functions with uniformly bound support can be shown to be an acceptable basis by this definition. The projection operators $\mathbf{P}^N$ associated with an acceptable basis have the form

$$\mathbf{P}^N := \sum_{m,n=1}^{N} \phi_m P_{mn} \phi_n^{\dagger}. \tag{2.10}$$

The $N \times N$ matrix, $\hat{P}$, with matrix elements P_{mn}, is

$$\hat{P} := \hat{O}^{-1}, \tag{2.11}$$

where the matrix elements of $\hat{O}$ are

$$O_{mn} = (\phi_m, \phi_n). \tag{2.12}$$

This matrix is the identity if the basis is orthonormal. It is always nonsingular because $\{\phi_n\}_{n=1}^{\infty}$ is a basis.

These projectors are used to construct finite rank approximations to each of the operators in Eqs. (2.5) and (2.6). The finite rank operators are defined as

$$\mathbf{V}^N = \mathbf{P}^N \mathbf{V} \mathbf{P}^N \tag{2.13}$$

$$\mathbf{M}^{2N} = \mathbf{P}^N [\mathbf{M}^2]\, \mathbf{P}^N. \tag{2.14}$$

These operators can be expressed in terms of the $N \times N$ matrices $\hat{V}$ and $\hat{M}^{2N}$, whose matrix elements are

$$V_{mn}^N := (\phi_n, V\phi_m) \tag{2.15}$$

$$M_{mn}^{2N} := (\phi_n, 4(-\nabla^2 + m^2)\, \phi_n), \tag{2.16}$$

as

$$\mathbf{V}^N = \sum_{m,n}^{N} \phi_m (\hat{P}\hat{V}\hat{P})_{mn} \phi_n^\dagger \tag{2.17}$$

$$\mathbf{M}^{2N} = \sum_{m,n}^{N} \phi_m (\hat{P}\hat{M}^{2N}\hat{P})_{mn} \phi_n^\dagger. \tag{2.18}$$

The computation of the matrix elements (2.15) and (2.16) do not require the evaluation of square roots. The finite rank analog of $\mathbf{M}_0^{-1}$, which is denoted by $\mathbf{M}^{-1N}$, is defined as

$$\mathbf{M}^{-1N} = \sum_{m,n}^{N} \phi_m (\hat{P}\hat{M}^{-1N}\hat{P})_{mn} \phi_n^\dagger, \tag{2.19}$$

where

$$\hat{M}^{-1N} = \hat{O}^{1/2} (\hat{P}^{1/2}\hat{M}^{2N}\hat{P}^{1/2})^{-1/2} \hat{O}^{1/2}. \tag{2.20}$$

The exponents $\frac{1}{2}$ indicate the square root of a positive definite Hermitian $N \times N$ matrix. Equation (2.20) is obtained by solving

$$\mathbf{M}^{-1N}\mathbf{M}^N = \mathbf{P}^N, \tag{2.21}$$

where

$$\mathbf{M}^N \cdot \mathbf{M}^N = \mathbf{M}^{2N} \tag{2.22}$$

subject to the condition that the range of these operators coincides with the range of $\mathbf{P}^N$.

To construct the approximate equation, assume that N is sufficiently large that the solution to Eq. (2.6) is well approximated by an expression of the form

$$\chi_N := \sum_{n}^{N} x_n \phi_n. \tag{2.23}$$

Equation (2.5) suggests that x_n be chosen so χ_N is the solution of the equation

$$(\mathbf{M}^{-1N} + \mathbf{M}^{-1N}\mathbf{V}^N\mathbf{M}^{-1N})\, \chi_N = \lambda_N (\mathbf{M}^{-1N})^2\, \chi_N. \tag{2.24}$$

This equation is equivalent to the following generalized eigenvalue problem for the eigenvalues λ_N and the coefficients $\vec{x}_N$,

$$(\hat{M}^{-1N} + \hat{M}^{-1N}\hat{P}\hat{V}\hat{P}\hat{M}^{-1N})\, \vec{x} = \lambda_N \hat{M}^{-1N}\hat{P}\hat{M}^{-1N}\vec{x}. \tag{2.25}$$

The approximate wave function appropriate to problem (2.1) is

$$\psi_N = \mathbf{M}^{-1N}\chi_N = \sum_{n}^{N} y_n \phi_n, \tag{2.26}$$

where

$$\vec{y} = \hat{P}\hat{M}^{-1N}\vec{x}. \tag{2.27}$$

The coefficients $\vec{y}$ are found using (2.27) in (2.25). The result is the equation

$$(\hat{I} + \hat{P}\hat{M}^{-1N}\hat{P}\hat{V})\,\vec{y} = \lambda_N \hat{P}\hat{M}^{-1N}\vec{y}. \tag{2.28}$$

The approximate equations are given by the pairs (2.23) and (2.25) or (2.27) and (2.28).

The general procedure for solving Eq. (2.1) is summarized below:

(1) Choose an acceptable basis (equivalently a set of projection operators satisfying (P1)–(P5).

(2) Choose $N < \infty$.

(3) Construct the matrices $\hat{O}$, $\hat{V}$, $\hat{M}^{2N}$ by computing the overlap integrals (2.12), (2.15), and (2.16).

(4) Construct $\hat{P}$, $\hat{M}^{-1N}$ using Eqs. (2.11) and (2.20).

(5) Construct the generalized eigenvalue problem (2.25) or (2.28) for the eigenvalues λ_N and the coefficients $\vec{x}$ or $\vec{y}$.

(6) Solve the generalized eigenvalue problem; construct the approximate eigenfunctions using (2.23) or (2.26).

It is important to note that this procedure only requires matrix elements of M^{2N} and V as input. Matrix elements of square roots of oprators are not needed. In general Eq. (2.1) will have a discrete spectrum and a continuous spectrum. In the next section it is shown that if λ_i is a discrete eigenvalue of (2.1) then there is a sequence of approximate eigenvalues λ_{N_i} with the property that $\lambda_{N_i} \to \lambda_N$. It follows that physical eigenvalues in the discrete spectrum can be identified by their stability with respect to increasing the number of basis functions.

The procedure outlined above can be simplified under a variety of circumstances. The first is to realize that Eq. (2.25) is algebraically equivalent to the equation

$$(\hat{O}\hat{M}^{1N}\hat{O} + \hat{V})\,\vec{y} = \lambda_N \hat{O}\vec{y}, \tag{2.29}$$

where

$$\hat{M}^{1N} = \hat{O}^{1/2}(\hat{P}^{1/2}\hat{M}^{2N}\hat{P}^{1/2})^{1/2}\,\hat{O}^{1/2}. \tag{2.30}$$

This is the equation that would be obtained if the procedure, used to obtain (2.25) from (2.5), were applied without regard for the boundedness of the operators. If the basis is orthonormal then the matrices $\hat{O}$ and $\hat{P}$ become the $N \times N$ identity matrix. Equations (2.29) and (2.30) are then replaced by

$$(\hat{M}^{1N} + \hat{V})\,\vec{y} = \lambda_N \vec{y} \tag{2.31}$$

and

$$\hat{M}^{1N} = (\hat{M}^{2N})^{1/2}. \tag{2.32}$$

3. CONVERGENCE

In this section it is proven that the oprators in Eq. (2.24) converge strongly to the operators in Eq. (2.5) when V is a bounded operator. This justifies the use of the finite rank treatment of the square root operator. This will be used to show that for each discrete eigenvalue, λ, of Eq. (2.5) there is a sequence of λ_N's that are eigenvalues of (2.24) with the property that $\lambda_N \to \lambda$ as $N \to \infty$.

The first step is to show that $\mathbf{M}^{-1N}$ converges strongly to $\mathbf{M}_0^{-1}$. This result is expressed by

THEOREM. *Let* $\mathbf{M}^{-1N}$ *be defined by* (2.19), *where* $\{\mathbf{P}^N\}_{N=1}^{\infty}$ *satisfies* (P1)–(P5). *Then for every* $\psi \in L^2(\mathbb{R}^3)$, *we have*

$$\lim_{N\to\infty} \|(\mathbf{M}^{-1N} - \mathbf{M}_0^{-1})\,\psi\| = 0. \tag{3.1}$$

This theorem is a consequence of the lemmas:

LEMMA 1. *Let* $\{\mathbf{P}^N\}_{N=1}^{\infty}$ *satisfy* (P1)–(P5) *and let* $\mathbf{M}^{2N}$ *be defined by* (2.14). *For every* ψ *satisfying* $\|\mathbf{M}_0^2\psi\| < \infty$, *we have*

$$\lim_{N\to\infty} \|(\mathbf{M}^{2N} - \mathbf{M}_0^2)\,\psi\| = 0 \tag{3.2}$$

LEMMA 2. *Let* $\{\mathbf{P}^N\}_{N=1}^{\infty}$ *satisfy* (P1)–(P5) *and let* $\mathbf{M}^{2N}$ *be defined by* (2.14). *For every* $\psi \in L^2(\mathbb{R}^3)$, *it follows that*

$$\lim_{N\to\infty} \|[(\mathbf{M}^{2N} \pm i)^{-1} - (\mathbf{M}_0^2 \pm i)^{-1}]\,\psi\| = 0. \tag{3.3}$$

To prove Lemma 1 note that for $\psi \in D(\mathbf{M}_0^2)$ that

$$\|(\mathbf{M}^{2N} - \mathbf{M}_0^2)\,\psi\| \leqslant \|\mathbf{M}_0^2(\mathbf{P}^N - 1)\,\psi\| + \|(1 - \mathbf{P}^N)\,\mathbf{M}_0^2\psi\|. \tag{3.4}$$

The first term on the right-hand side vanishes as $N \to \infty$ by (P5) because $\psi \in D(\mathbf{M}_0^2)$. The second term vanishes because $\|\mathbf{M}_0^2\psi\| < \infty$. This proves Lemma 1.

To prove Lemma 2 let let $\alpha = \pm i$, $\psi \in L^2(\mathbb{R}^3)$ and use the second resolvent relations to obtain

$$\|[(\alpha + \mathbf{M}^{2N})^{-1} - (\alpha + \mathbf{M}_0^2)^{-1}]\,\psi\| \leqslant \|(\mathbf{M}^{2N} - \mathbf{M}_0^2)\,\xi\|, \tag{3.5}$$

where

$$\xi = [(\alpha + \mathbf{M}_0^2)^{-1}]\,\psi \tag{3.6}$$

since $\|\mathbf{M}_0^2\xi\| \leqslant (\text{const.})\|\psi\| < \infty$, the desired result follows by applying Lemma 1 to the right-hand side of (3.5). This proves Lemma 2.

The theorem is proven by combining Lemma 2 with the Weierstrass approximation theorem [8]. To do this define the continuous function

$$f(y) := \frac{2m\sqrt{1+y}}{[1+16m^4+\sqrt{(1+16m^2)^2-(1+y)^2\,16m^4}]^{1/2}} \tag{3.7}$$

on $[-1, 1]$. This function is obtained by solving

$$y = -1 + \frac{1+16m^4}{4m^2}\left(\frac{1}{x+1}+\frac{1}{x-i}\right) \tag{3.8}$$

for $x^{-1/2}$ as a function of y. By the Weierstrass approximation theorem there are coefficients a_n such that

$$\left| f(y) - \sum_{n=0}^{M} a_n\, y^n \right| < \varepsilon(M) \tag{3.9}$$

for all $y \in [-1, 1]$. It follows that

$$\| f(\mathbf{Y}) - \sum_{n=0}^{M} a_n(\mathbf{Y})^n \| < \varepsilon(M) \tag{3.10}$$

for

$$\mathbf{Y} = \mathbf{Y}_0 = -1 + \frac{1+16m^4}{4m^2}\left(\frac{1}{\mathbf{M}_0^2+i}+\frac{1}{\mathbf{M}_0^2-i}\right) \tag{3.11}$$

and

$$\mathbf{Y} = \mathbf{Y}_N = -1 + \frac{1+16m^4}{4m^2}\left(\frac{1}{\mathbf{M}^{2N}+i}+\frac{1}{\mathbf{M}^{2N}-i}\right) \tag{3.12}$$

since in both cases of $\sigma(\mathbf{Y}) \in [-1, 1]$. It is important to note that the bound in (3.9) is independent of the N in (3.12). To prove the theorem observe that

$$\begin{aligned}
&\|(\mathbf{M}^{-1N} - \mathbf{M}_0^{-1})\,\psi\| \\
&\quad = \|(f(\mathbf{Y}_N) - f(\mathbf{Y}_0))\,\psi\| \\
&\quad \leqslant \left\| \left(f(\mathbf{Y}_N) - \sum_{n=0}^{M} a_n(\mathbf{Y}_N)^n \right)\psi \right\| + \sum_{n=0}^{M} a_n n\, \|(\mathbf{Y}_N - \mathbf{Y}_0)\,\psi\| \\
&\qquad + \left\| \left(f(\mathbf{Y}_0) - \sum_{n=0}^{M} a_n(\mathbf{Y}_0)^n \right)\psi \right\|,
\end{aligned} \tag{3.13}$$

where the last step follows because $\|\mathbf{Y}_0\|$, $\|\mathbf{Y}_N\| \leqslant 1$. The first and last terms in (3.13) can be made arbitrarily small by (3.10) while the middle term can be made arbitrarily small by Lemma 2. This proves the theorem.

It follows from the theorem and the fact that $\mathbf{V}$ is bounded that the operators in (2.24) strongly converge to the operators in (2.5).

Next the implications of this strong convergence on the eigenvalue spectrum and the eigenfunctions are considered when λ_0 is a discrete eigenvalue of Eq. (2.1) with eigenfunction ψ_0. Equations (2.5) and (2.6) are rewritten as

$$(1+\mathbf{M}_0^{-1}\mathbf{V})\,\psi_0=\lambda_0\mathbf{M}^{-1}\psi_0. \tag{3.14}$$

Assume that $\{\lambda_N^n\}$ and $\{\psi_N^n\}$ are solutions of the corresponding finite rank equation

$$(\mathbf{P}^N+\mathbf{M}^{-1N}\mathbf{V}^N)\,\psi_N^n=\lambda_N^n\mathbf{M}^{-1N}\psi_N^n. \tag{3.15}$$

The solutions of (3.15) are chosen to be orthonormal. These equations have the form

$$\mathbf{A}\psi_0=\lambda_0\mathbf{B}\psi_0 \tag{3.16}$$

and

$$\mathbf{A}^N\psi_N^n=\lambda_N^n\mathbf{B}^N\psi_N^n, \tag{3.17}$$

respectively. ψ_0 can be expanded in terms of the ψ_N^n to obtain

$$\psi_N^0=\sum_{n=1}^{N}a_n\psi_N^n, \tag{3.18}$$

and compute

$$\|(\mathbf{A}^N-\lambda_0\mathbf{B}^N)\,\psi^0\|=\left[\sum_{n=1}^{N}|a_n|^2\,(\lambda_N^n-\lambda_0)^2\right]^{1/2}. \tag{3.19}$$

If this is combined with (3.16), we obtain

$$\begin{aligned}\|(\mathbf{A}^N-\lambda_0\mathbf{B}^N)\,\psi_0\|&=\left[\sum_{n=1}^{N}|a_n|^2\,(\lambda_N^n-\lambda_0)^2\right]^{1/2}\\&\leqslant\|(\mathbf{A}-\mathbf{A}^N)\,\psi_0\|+|\lambda_0|\,\|(\mathbf{B}-\mathbf{B}^N)\,\psi_0\|.\end{aligned} \tag{3.20}$$

The right-hand side necessarily vanishes as $N\to\infty$ as a result of the theorem. If we let $\lambda_N^{n'}$ be the eigenvalue that minimizes $|(\lambda_N^{n'}-\lambda_0)|$, we obtain

$$|\lambda_N^{n'}-\lambda_0|\leqslant\frac{(\|(\mathbf{A}-\mathbf{A}^N)\,\psi_0\|+|\lambda_0|\,\|(\mathbf{B}-\mathbf{B}^N)\,\psi_0\|)}{\|\mathbf{P}^N\psi_0\|} \tag{3.21}$$

which clearly vanishes as $N\to\infty$. Thus at least one of the eigenvalues of the approximate eigenvalue problem can be made arbitrarily close to one of the exact

eigenvalues by choosing N sufficiently large. If (3.20) and (3.21) are combined we obtain

$$\|(\mathbf{A}^N - \lambda_N^{n'}\mathbf{B}^N)\,\psi_0\| \leqslant \|(\mathbf{A}-\mathbf{A}^N)\,\psi_0\|\left(1+\frac{\|\mathbf{B}\psi_0\|}{\|\mathbf{P}^N\psi_0\|}\right)$$
$$+\|(\mathbf{B}-\mathbf{B}_N)\,\psi_0\|\left(|\lambda_N|+|\lambda_0|\,\frac{\|\mathbf{B}\psi_0\|}{\|\mathbf{P}^N\psi_0\|}\right). \tag{3.22}$$

The right-hand side of this expression can be made arbitrarily small by taking N sufficiently large. Thus the solution ψ_0, to (3.14), satisfies the finite rank equation (3.15) to any desired accuracy for some $\lambda_N^{n'}$ and sufficiently large N.

It is useful to summarize the three main results of this section. First, the operators in the finite rank equaton (2.25) converge strongly to the operators in (2.5). Second, to each discrete eigenvalue of Eq. (2.5), there is an eigenvalue of (2.25) that is arbitrarily close to λ_0 for sufficiently large N. Third, each discrete eigenfunction, ψ_0, of (3.16) satisfies (3.17) to any desired accuracy for some $\lambda_N^{n'}$ with sufficiently large N.

4. Variational Methods

In this section it is shown how the results of the last section can be improved when $\{\phi_n\}_{n=1}^{\infty}$ represents an acceptable basis that is easily Fourier transformed. In this case $\mathbf{M}_0^{-1}$ is a multiplication operator in the momentum representation. Because of this it is possible to construct approximate finite rank approximations by taking matrix elements of the operators in (2.5) directly. This method has been previously applied by Stanley and Robson [7] using a harmonic oscillator basis. In this case Eq. (2.25) is replaced by

$$\sum_{m=1}^{N}(\chi_n, [\mathbf{M}_0^{-1}+\mathbf{M}_0^{-1}\mathbf{V}\mathbf{M}_0^{-1}]\,\chi_m)\,x_m = \sum_{m=1}^{N}\lambda(\chi_n, \mathbf{M}_0^{-2}\chi_m)\,x_m \tag{4.1}$$

$$\psi = \sum_{n=1}^{N} x_n\phi_n = \sum_{n=1}^{N} x_n(2\sqrt{\vec{k}^2+m^2})^{-1}\,\chi_n. \tag{4.2}$$

The theorem of Section 3 also applies to Eq. (4.1). The operators in (4.1) all converge strongly to their exact counterparts. The other results of Section 3 also hold when $\mathbf{M}_0^{-1}$ is absorbed into the wave function from the left of (4.1).

Equation (4.1) has two additional features. This first is that the lowest k eigenvalues of (4.1) are variational upper bounds on the lowest k eigenvalues of (2.5). This property is not realized in the method of Section 3. The second property is that if ψ_0 is the eigenvector of (2.5) with the kth smallest eigenvalue, λ_k, and ϕ_N^l is

the eigenvector of (4.1) and (4.2), $[\phi_N^l = (2\sqrt{k^2+m^2})^{-1}\,\chi_N^l]$ with the lth smallest eigenvalue, then

$$\lim_{N\to\infty}(\phi_N^l, \psi_0) = 0 \qquad (l \neq k). \tag{4.3}$$

To show that the lowest k eigenvalues of (4.1) are variational upper bounds on the lowest k discrete eigenvalues of (2.5), fix N and let $\{\xi_n\}_{n=1}^N$ be solutions of (4.1) with eigenvalues λ_N^n. Let ξ be any linear combination of the ξ_m's;

$$\xi = \sum_{m=1}^{N} a_m \xi_m.$$

Then

$$\frac{(\xi, [\mathbf{M}_0^{-1} + \mathbf{M}_0^{-1}\mathbf{V}\mathbf{M}_0^{-1}]\,\xi)}{(\xi, \mathbf{M}_0^{-2}\xi)} = \frac{\sum_{m=1}^N |a_m|^2 \lambda_m}{\sum_{m=1}^N |a_m|^2} \geqslant (\lambda_m)_{\min}$$

$$\geqslant \inf_{\xi} \frac{(\xi, [\mathbf{M}_0^{-1} + \mathbf{M}_0^{-1}\mathbf{V}\mathbf{M}_0^{-1}]\,\xi)}{(\xi, \mathbf{M}_0^{-2}\xi)} = \lambda_0, \tag{4.4}$$

where λ_0 is the smallest eigenvalue of (2.5). Thus the lowest eigenvalue of the approximate problem is a variational upper bound on λ.

To extend this principle to the lowest k eigenvalues of (2.5) the functional

$$\Lambda(\xi) = \frac{(\xi, [\mathbf{M}_0^{-1} + \mathbf{M}_0^{-1}\mathbf{V}\mathbf{M}_0^{-1}]\,\xi)}{(\xi, \mathbf{M}_0^{-2}\xi)} \tag{4.5}$$

is defined. The first k eigenvectors of (4.1) span a k dimension linear space on which the functional $\Lambda(\xi)$ is at or below the maximum of these k eigenvalues. Thus the linear space

$$\{\xi \,|\, \Lambda(\xi) \leqslant \lambda_k\} \tag{4.6}$$

is at least k dimensional. Thus Eq. (2.5) must have at least k eigenvalues with values less than or equal to the largest of the $\{\lambda_n\}_{n=1}^k$.

These variational bounds can be combined with Eq. (3.20) to obtain

$$\lim_{N\to\infty}\left[\sum_{n=1}^{N} |a_n^N|^2 (\lambda_N^n - \lambda_0)^2\right]^{1/2} = 0. \tag{4.7}$$

This means that for every $\varepsilon > 0$, there is an N such that

$$|a_n^N| = |(\psi_N^n, \psi_0)| \leqslant \frac{\varepsilon}{|\lambda_N^n - \lambda_0|}. \tag{4.8}$$

This result holds for the equations of Section 2. The variational bounds on the eigenvalues guarantee that for sufficiently large N the denominators are uniformly

bound away from 0, except for the case when $n=m$, where λ_0 is the mth smallest eigenvalue of (2.5). This shows that

$$\lim_{N\to\infty} a_n^N = 0 \qquad \text{if} \quad n \neq m \tag{4.9}$$

which is the other main result of this section. These results apply to the technique used in Ref. [7] provided the basis satisfies condition (P5).

5. Coulomb, Yukawa, and Confining Potentials

The situation that the potential $\mathbf{V}$ is a bounded operator does not include some of the cases of most physical interest. Two different types of unbounded potentials are frequently encountered in applications. The first occurs when the potential has a $1/r$ singularity at the origin. This occurs in the case of Coulomb interactions, Yukawa-like strong interactions, and quark–antiquark interactions. A second class of physically interesting potentials is confining interactions such as the linear and harmonic oscillator potentials. These potentials arise in problems related to quark confinement.

We first consider the case of the $1/r$ singularity. From a theoretical point of view, this type of potential might be expected to cause difficulties. It is known that the combination of the $1/r$ potential and the square root operator lead to singular behavior at the origin [9]. In our approach the $1/r$ potential causes no special problems. What makes the $1/r$ potential nice is that even though $\mathbf{V}_c$ is unbounded,

$$\mathbf{M}_0^{-1}\mathbf{V}\mathbf{M}_0^{-1} \tag{5.1}$$

is bounded. This means that the finite rank approximations based on Eq. (4.1) converge strongly to the exact Eq. (2.5). The variational bounds of the previous section also hold.

To show that $\mathbf{M}_0^{-1}\mathbf{V}\mathbf{M}_0^{-1}$ is bounded for a $1/r$ potential, let

$$V(r) = \frac{f(r)}{r}, \tag{5.2}$$

where $f(r)$ is bounded. $V(r)$ is rewritten as

$$V(r) = \left(\frac{f(r)}{r} - \frac{f(0)}{r}e^{-Br}\right) + f(0)\frac{e^{-Br}}{r}$$

$$= V_B(r) + f(0)\, V_y(r). \tag{5.3}$$

$V_B(r)$ is bounded. It is shown that $\mathbf{M}_0^{-1} V_y(r) \mathbf{M}_0^{-1}$ is Hilbert-Schmidt (HS) [10] and consequently bounded:

$$|||\mathbf{M}_0^{-1}\mathbf{V}_y\mathbf{M}_0^{-1}||| \leqslant |||M_0^{-1}V_yM_0^{-1}|||_{\mathrm{HS}} = \left[\frac{1}{2\pi^2}\int \frac{1}{4(k^2+m^2)} \times \frac{d^3R}{(k-k')^2+B^2}\frac{d^3R'}{4(k')^2+m^2}\frac{1}{(k-k')^2+B^2}\right]^{1/2} < \infty. \quad (5.4)$$

This shows that $\mathbf{M}_0^{-1}\mathbf{V}\mathbf{M}_0^{-1}$ is a bounded operator. This analysis shows that Coulomb-like singularities can be treated with Eq. (4.1).

The second class of unbounded potentials of interest are the confining potentials. To render these in a form amenable to strongly convergent approximations, we let γ be a constant such that

$$\gamma + V > 0. \quad (5.5)$$

Equation (2.1) may be rewritten in the form

$$\left(\mathbf{M}_0^{-1}\frac{1}{\gamma+V} + \mathbf{M}_0^{-1}\frac{V}{\gamma+V}\mathbf{M}_0^{-1}\right)\chi = \mathbf{M}_0^{-1}\frac{\lambda}{\gamma+V}\mathbf{M}_0^{-1}\chi \quad (5.6)$$

$$\psi = \mathbf{M}_0^{-1}\chi. \quad (5.7)$$

The approximation theorem of Section 3 is still valid for $\mathbf{M}_0^{-1}$. Finite rank approximations to $V/(\gamma+V)$ and $(\gamma+V)^{-1}$ can be computed directly. This equation can be discretized as in Sections 3 or 4. The results of Sections 3 and 4 hold.

In numerical applications we found that it was not necessary to make the transformation (5.6) to obtain reliable numerical solutions.

6. Numerical Tests

In this section the computational methods discussed in this paper are tested. The method of Sections 2–4 is applied to solving the equations

$$\left(2[m^2-\nabla^2]^{1/2} - \frac{C_1}{r}\right)\psi = \mu\psi \quad (6.1)$$

and

$$\left(2[m^2-\nabla^2]^{1/2} - \frac{C_1}{r} + C_2 r\right)\psi = \mu\psi. \quad (6.2)$$

The parameters used are $m = 0.313$ GeV, $C_1 = 0.5$, and $C_2 = 0.197$ (GeV)^2. These parameters are chosen so that we can compare our results for Eq. (6.2) with the results of Ref. [6]. Calculations for (6.1) do not exist. The choice $C_1 = 0.5$ is interesting because it leads to a strong Coulomb field where one anticipates more

numerical difficulties. In this case calculations based on the method of Section 2 are compared to variational calculations of Section 4.

Equation (2.28) is used to compute the eigenvalues where the basis functions are

$$\psi_n(\vec{r}) = \frac{1}{r^\alpha} S_n(r)\, e^{-r/r_1} Y_{LM}(\hat{r}). \tag{6.3}$$

The functions $S_n(r)$ are de Boors B-splines [11]. They are piecewise polynomials of degree 3 that have compact support and one continuous derivative everywhere. This choice has not been checked to see if it leads to a set of projection oprators $\{P^N\}$ satisfying (P5). The coefficient α allows us to include singularities in our basis functions that are expected from theoretical considerations [9].

Equation (4.1) is solved for the variational calculations using the basis

$$\phi_n(\vec{r}) = N_n r^{n-\alpha} e^{-\beta r} Y_{00}(\hat{r}) \tag{6.4}$$

$$N_n = \frac{(2\beta)^{n-\alpha+3/2}}{\sqrt{\Gamma(2n-2\alpha+3)}} \tag{6.5}$$

which have the Fourier transforms

$$\tilde{\phi}_n(\vec{k}) = \sqrt{2/\pi}\, \frac{N_n}{|\vec{k}|}\, \Gamma(n+2-\alpha)(\beta^2+\vec{k}^2)^{-(n+2-\alpha)/2}$$

$$\times \sin\left[(n+2-\alpha)\tan^{-1}\left(\frac{k}{\beta}\right)\right] \hat{Y}_{00}(\hat{k}). \tag{6.6}$$

Matrix elements of both potentials in (6.1) and (6.2) can be computed analytically in this basis. The results are

$$V^L_{nm} = -C_1 N_n N_m \left(\frac{1}{2\beta}\right)^{n+m-2\alpha+2} \Gamma(n+m-2\alpha+2) \tag{6.7}$$

for the Coulomb potential and

$$V^L_{nm} = C_2 N_m N_m \left(\frac{1}{2\beta}\right)^{n+m-2\alpha+4} \Gamma(n+m-2\alpha+4) \tag{6.8}$$

for the linear potential. The matrix elements of $\mathbf{M}_0^2$ are computed numerically in this basis using the following points and weights in momentum space

$$k_m = \beta \tan\left(\frac{2m-1}{2N}\pi\right) \tag{6.9}$$

$$\omega_m = \frac{\pi}{2N\beta}(k_m^2+\beta^2). \tag{6.10}$$

These integrate polynomials of degree $\leqslant 2N$ in $1/(k^2+\beta^2)$ exactly.

The results of the numerical calculations of the eigenvalues of Eqs. (6.1) and (6.2) are shown in Tables I–X. Tables I–IV show the results of four different calculations

TABLE I

NS	$N=0, L=0$	$N=1, L=0$	$N=2, L=0$
8	0.605488	0.621530	0.624438
12	0.605348	0.621208	0.624169
16	0.605323	0.621074	0.624011
20	0.605299	0.621012	0.623919
24	0.605184	0.620979	0.623865
28	0.605244	0.620958	0.623833
32	0.605143	0.620944	0.623813
36	0.605130	0.620934	0.624018

Note. $CC=-0.5$, $m=0.313$ GeV, $\alpha=0$.

TABLE II

N	$N=0, L=0$	$N=1, L=0$	$N=2, L=0$
5	0.605242	0.620897	0.623848
6	0.605214	0.620894	0.623773
7	0.605193	0.620892	0.623763
8	0.605177	0.620890	0.623756

Note. $CC=-0.5$, $m=0.313$ GeV, $\alpha=0$.

TABLE III

NS	$N=0, L=0$	$N=1, L=0$	$N=2, L=0$
8	0.606037	0.621333	0.624366
12	0.605798	0.621148	0.624088
16	0.605648	0.621103	0.623940
20	0.605548	0.621081	0.623868
24	0.605477	0.621062	0.623837
28	0.605477	0.621044	0.623823
32	0.605379	0.621028	0.623817
36	0.605389	0.621014	0.623813

Note. $CC=-0.5$, $m=0.313$ GeV, $\alpha=0.191$.

TABLE IV

N	$N=0, L=0$	$N=1, L=0$	$N=2, L=0$
5	0.60506565	0.62087646	0.62384916
6	0.60506341	0.62087625	0.62377917
7	0.60506232	0.62087616	0.62375772
8	0.60506178	0.62087611	0.62375329

Note. $CC=-0.5$, $m=0.313$ GeV, $\alpha=0.191$.

TABLE V

NS	$N=0, L=0$	$N=1, L=0$	$N=2, L=0$
8	1.420849	2.130627	2.682589
12	1.419318	2.114944	2.649517
16	1.418860	2.111962	2.637593
20	1.418620	2.111215	2.634497
24	1.418466	2.110905	2.633593
28	1.418318	2.110654	2.633116
Ref. [6]	1.43		

Note. $CC=-0.5$, $CL=0.197$ (GeV)^2, $m=0.313$ GeV.

of the first three $L=0$ eigenvalues of Eq. (6.1). Tables V–X show the results of calculations of the $N\leqslant 3$, $L\leqslant 4$ eigenvalues of Eq. (6.2). Tables XI and XII illustrate the use of the methods introduced in this paper to estimate the size of relativistic effects in models of light quarks.

Tables I and III utilize the method outlined in Section 2. The functions in Eq. (6.3) are used as a basis. The splines are such that only four of the functions $S_n(r)$ are nonzero between any adjacent pair of breakpoints. We use a finite number of equally spaced breakpoints on an interval [0, RMAX]. The number of splines

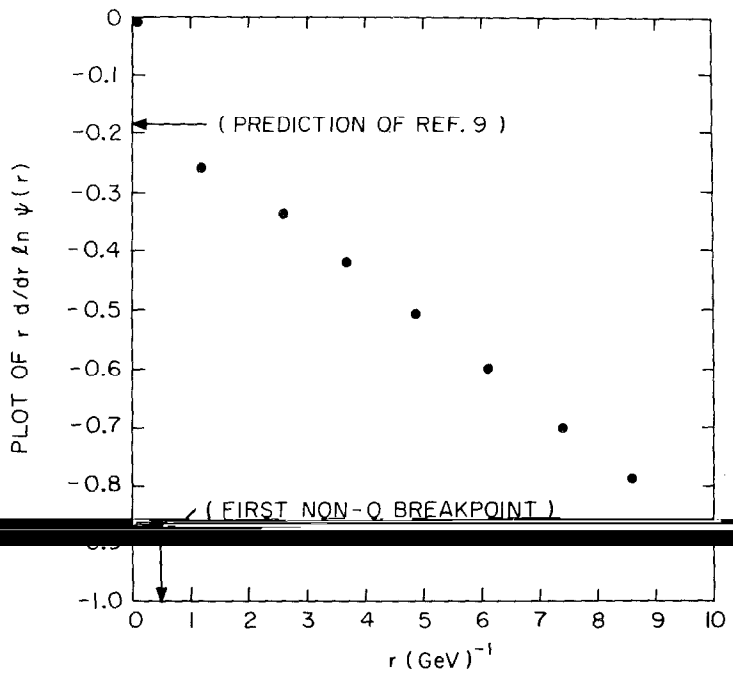

FIG. 1. Singular behavior of the relativistic ground-state Coulomb wave function.

TABLE VI

N	$N=0, L=0$	$N=1, L=0$	$N=2, L=0$
5	1.418778	2.124193	2.689752
6	1.418698	2.117667	2.689520
7	1.418698	2.113101	2.675678
8	1.418657	2.111703	2.654051
Ref. [6]	1.43		

Note. $CC=-0.5$, $CL=0.197$ (GeV)^2, $m=0.313$ GeV.

(NS) that appear in the tables is related to the number of breakpoints (NB) by NS = 2 NB − 2. Convergence is tested by increasing the number of breakpoints. Equally spaced breakpoints are not the best choice for calculations, however, they allow for a systematic study of the convergence properties. Because the eigenfunctions for different values of the principal quantum number N are so different, it was necessary to use a different value of r_1 and RMAX to compute each of the columns of Tables I and III. The values of r_1 were chosen to be the approximate RMS separation between the particles in the eigenstate in question. The value of RMAX was chosen to be a distance after which the wave function had fallen at least four orders of magnitude below its maximal value. The parameter r_1 and RMAX are $r_1 = 20.72$, 80, 170 (GeV) and RMAX = 120, 400, 700 (GeV) for $N=0$, 1, and 3, respectively. The calculations in these two tables differ in the value of the parameter α. Reference [9] predicts that for r near the origin, the ground-state wave function behaves like (6.3) with $\alpha = 0.191$ (for this choice of CC). (The eigenvalue spectrum predicted in Ref. [9] is known to be incorrect [12] and does not agree with our results.) The calculations in Table I have $\alpha = 0$ while those in Table III have $\alpha = 0.191$.

The other two tables use the variational method discussed in Section 4. They use the basis (6.4) with $1/\beta = 20$ (GeV). For this calculation it is sufficient to work with

TABLE VII

NS	$N=0, L=1$	$N=1, L=1$	$N=2, L=1$
8	1.940474	2.526819	3.092469
12	1.936778	2.481394	2.949761
16	1.936569	2.478867	2.930741
20	1.936479	2.478702	2.929350
24	1.936437	2.478557	2.929210
28	1.936419	2.478470	2.929036
Ref. [6]	1.94		

Note. $CC=-0.5$, $CL=0.197$ (GeV)^2, $m=0.313$ GeV.

TABLE VIII

NS	$N=0, L=2$	$N=1, L=2$	$N=2, L=2$
8	2.329840	2.808288	3.303489
12	2.321951	2.793779	3.203620
16	2.318731	2.786015	3.193245
20	2.317956	2.782553	3.188516
24	2.317770	2.781409	3.185776
28	2.317716	2.781061	3.184693
Ref [6]	2.32		

Note. $CC=-0.5$, $CL=0.197$ (GeV)^2, $m=0.313$ GeV.

one value of β for $N=0$, 1, and 2. Tables II and IV show the result of this calculation for different numbers of basis functions with $\alpha=0$ and $\alpha=0.191$, respectively. This calculation has the advantage that the eigenvalues are variational bounds on the exact eigenvalues. They also provide a good consistency of the calculation in Tables I and III. The results of all four are consistent. The inclusion of a nonzero α has a 0.03% effect on the ground-state eigenvalue in the variational calculations. It results in a lowering of the variational energy.

An interesting question is whether there is any numerical evidence of the singular behavior of the wave function prediced in [9]. The configuration space splines have the advantage that they are localized in configuration space. Even though a basis with $\alpha=0$ cannot possibly be used to accurately represent a function with a non-integer value of α near the origin, if we put a few breakpoints near the origin the desired behavior should appear near the origin. In this case near is defined as a distance beyond a few breakpoints. To test this we calculate $r\ d/dr\ \ln[\psi(r)]$ as a function of r for points near the origin but beyond the first two breakpoints, where ψ is the ground-state solution of (6.1) with $\alpha=0$. The results of this calculation are plotted in Fig. 1. If we extrapolate the curve that goes through these points to the origin, we obtain an estimate for α. The prediction of Ref. [9] is consistent with the calculations in Fig. 1, which suggest a value of α between -0.15 and -0.2.

TABLE IX

NS	$N=0, L=3$	$N=1, L=3$	$N=2, L=3$
8	2.662795	3.1012672	3.496928
12	2.642299	3.067238	3.461868
16	2.640033	3.053762	3.427641
20	2.639883	3.051394	3.421447
24	2.639872	3.051139	3.419517
28	2.639862	3.051107	3.419289
Ref. [6]	2.65		

Note. $CC=-0.5$, $CL=0.197$ (GeV)^2, $m=0.313$ GeV.

TABLE X

NS	$N=0, L=4$	$N=1, L=4$	$N=2, L=4$
8	2.946010	3.394339	3.732608
12	2.925921	3.306771	3.672389
16	2.925330	3.299750	3.644594
20	2.925285	3.298824	3.640246
24	2.925230	3.298865	3.639646
28	2.925204	3.298771	3.639590
Ref. [6]	2.93		

Note. $CC=-0.5$, $CL=0.197$ (GeV)^2, $m=0.313$ GeV.

The calculations in Tables V–X are for Eq. (6.2). Spline and variational calculations are presented for the case $L=0$ in Tables V and VI. In this example each table uses a single value of r_1 and RMAX. In all of these calculations we have set $\alpha=0$. Spline calculations are also performed for $L=1$, 2, 3, and 4. We chose these values because other variational Monte Carlo calculations [6] exist for these values of L. The values of r_1 and RMAX used for $L=1$, 2, 3, 4 are 3, 5, 6, 7.5, 8 (GeV) and 20, 22, 24, 25, 26 (GeV), respectively. The variational calculations in Table VI are for $1/\beta=20$ (GeV). Both calculations in Tables V and VI are in good agreement with the results of Ref. [6] and with each other. The spline calculations in Tables VII–X are also in good agreement with the calculations of Ref. [6]. We were unable to find analytic Fourier transforms of the functions (6.4) for values of $L>0$ so we did not do variational calculations for nonzero values of L.

The calculation of relativistic corrections to the kinetic energy for systems of light quarks is a typical application of the methods introduced in this paper. This can be done by comparing the mass eigenvalues of Eq. (6.2) with those of the corresponding nonrelativistic equation

$$\left(2m+\frac{k^2}{m}-\frac{C_1}{r}+C_2 r\right)\psi=\mu\psi.$$

TABLE XI

State	$N=0, L=0$	$N=1, L=0$	$N=2, L=0$
Eq. (6.9)	1.643[a]	2.608[a]	3.374[a]
Eq. (6.2)	1.418[a]	2.110[a]	2.633[a]
$\Delta\mu$	0.225[a]	0.498[a]	0.741[a]
$\frac{\Delta\mu}{m}$	0.72	1.59	2.37

[a] In GeV.

TABLE XII

State	$(N=0, L=0)-(N=0, L=0)$	$(N=2, L=0)-(N=1, L=0)$
Eq. (6.9)	0.965[a]	0.766[a]
Eq. (6.2)	0.692[a]	0.523[a]
$\Delta\mu$	0.273[a]	0.243[a]
$\frac{\Delta\mu}{m}$	0.87	0.78

[a] In GeV.

We compare the results of these two calculations in Tables XI and XII. Both calculations use $m=0.313$ GeV, $C_1=0.5$, and $C_2=0.197$ (GeV)^2. Table XI compares the difference in the eigenvalues obtained from these two equations in the first three states. These differences are compared to the mass of the quark. Table XII does the same thing for the splittings between energy levels. In both sets of calculations we see large relativistic effects.

In this paper we have devised new numerical methods for solving eigenvalue problems with square root operators. This was done in two steps. The first was to reformulate the equation into an equation involving only bounded operators. The second step is to make strong finite rank approximations to these operators. Specific calculations are performed based on the methods introduced in Sections 3 and 4. The results of the two calculations are consistent with each other and consistent with the results of Ref. [6]. The main conclusion is that for a basis that satisfies condition (P5), a finite rank treatment of square root operators involving an eigenvalue problem is justified.

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