

Nystrom plus correction method for solving bound-state equations in momentum space

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A method is presented for solving the momentum-space Schrödinger equation with a linear potential. The Lande-subtracted momentum-space integral equation can be transformed into a matrix equation by the Nystrom method. The method produces only approximate eigenvalues in the cases of singular potentials such as the linear potential. The eigenvalues generated by the Nystrom method can be improved by calculating the numerical errors and adding the appropriate corrections. The end results are more accurate eigenvalues than those generated by the basis function method. The method is also shown to work for a relativistic equation such as the Thompson equation.

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I. INTRODUCTION

The momentum-space Schrödinger equation has a singular kernel for both the Coulomb and linear potentials. The Coulomb singularity is removed with the Lande-subtraction method [1,2]. Previous work [3–5] showed how to remove the singularity from the linear potential using a subtraction method with basis functions. A problem with this method is that one must guess a suitable set of basis functions in advance. In this paper, we show that Nystrom method [7] can solve the same problem more simply and accurately. We begin with a review of the basis function method. Then we introduce the Nystrom method and apply it to the s -state momentum-space Schrödinger equation with a linear potential. We use our new numerical results to show that the Nystrom plus correction method is more accurate than the basis function method. At the end, we generalize the Nystrom method to higher angular momentum quantum numbers ($l > 0$).

II. BASIS FUNCTION METHOD

We begin this paper with a discussion of the basis function method to give the proper theoretical motivation. We shall use the simplest momentum-space Schrödinger equation to illustrate the principles of the numerical methods, which is the s -state equation.

The momentum-space Schrödinger equation is related to an integral equation of the Fredholm type

$$\int K(p, p') \phi(p') dp' = \lambda \phi(p). \quad (1)$$

Suppose that the wave function ϕ can be expanded in a set of basis functions $\{g_i\}$, such that

$$\phi(p) = \sum_{i=1}^N C_i g_i(p), \quad (2)$$

where C_i are constant coefficients. Substitute Eq. (2) into Eq. (1) to obtain

$$\sum_{i=1}^N \int K(p, p') C_i g_i(p') dp' = \lambda \sum_{i=1}^N C_i g_i(p). \quad (3)$$

Now multiply both sides of Eq. (3) with $g_j(p)$ and integrate over p to symmetrize the equation over i and j ,

$$\sum_{i=1}^N C_i \underbrace{\int \int K(p, p') g_i(p') g_j(p) dp' dp}_{A_{ij}} = \lambda \sum_{i=1}^N C_i \underbrace{\int g_i(p) g_j(p) dp}_{B_{ij}}, \quad (4)$$

and the result is a matrix equation,

$$\sum_{i=1}^N A_{ij} C_i = \lambda \sum_{i=1}^N B_{ij} C_i, \quad (5)$$

where C_i is the eigenvector and λ is the eigenvalue. The indices i and j correspond to the quadrature points p and p' . N represents the number of mesh points. In the case of the momentum-space Schrödinger equation with a Coulomb or linear potential, the kernel \mathbf{A} is singular. A simple example is the momentum-space Schrödinger equation with a linear potential in the S state [3,5],

$$\frac{p^2}{2\mu} \phi_{n0}(p) + \frac{\lambda_L}{\pi p^2} \int_0^\infty \underbrace{\left[\frac{\eta^2}{p'p} Q_0''(y) + Q_0'(y) \right]}_{V_0^L(p, p')} \times \phi_{n0}(p') dp' = E_{n0} \phi_{n0}(p), \quad (6)$$

where $y = (p^2 + p'^2)/2p'p$,

$$Q_0'(y) = p'p \left[\frac{1}{(p+p')^2 + \eta^2} - \frac{1}{(p-p')^2 + \eta^2} \right], \quad (7)$$

and

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$$\frac{\eta^2}{p'p} Q_0''(y) = \eta^2(p^2 + p'^2 + \eta^2) \times \left[\frac{1}{(p+p')^2 + \eta^2} - \frac{1}{(p-p')^2 + \eta^2} \right]^2. \quad (8)$$

Lande subtraction [3,5,6] involves subtracting a zero term

$$\int_0^\infty \left[\frac{\eta^2}{p'p} Q_0''(y) + Q_0'(y) \right] dp' = 0 \quad (9)$$

from Eq. (6) such that

$$\frac{p^2}{2\mu} \phi_{n0}(p) + \frac{\lambda_L}{\pi p^2} \int_0^\infty \left[\frac{\eta^2}{p'p} Q_0''(y) + Q_0'(y) \right] \times [\phi_{n0}(p') - \phi_{n0}(p)] dp' = E_{n0} \phi_{n0}(p). \quad (10)$$

Using Eqs. (7) and (8), the integral in Eq. (10) for $p > 0$ in the limit of $y \rightarrow 1$ can be shown to equal

$$\lim_{\eta \rightarrow 0} \lim_{p \rightarrow p'} \frac{\lambda_L}{\pi} \left[2\eta^2 \left\{ \frac{1}{(p-p')^2 + \eta^2} \right\}^2 - \frac{1}{(p-p')^2 + \eta^2} \right] \times (p-p')^2 \frac{d\phi_{n0}}{dp} = 0. \quad (11)$$

The order of the limits in Eq. (11) is important. The reverse order will lead to the nonsensical result $\int Q_0'(y) dp' = 0$. Next, in the limit of $p, p' \rightarrow 0$, $(p+p')^2 = (p-p)^2$. By substituting this equality into Eqs. (7) and (8), it can be shown again that the integral in Eq. (10) vanishes for $p \rightarrow 0$ at $y = 1$. At the end, the integral vanishes at $y = 1 \forall p$. Away from the singularities, both integrands in the integral of Eq. (10) are finite. By taking $\eta \rightarrow 0$, the first integrand vanishes. The final form of Eq. (10) is

$$\frac{p^2}{2\mu} \phi_{n0}(p) + \frac{\lambda_L}{\pi p^2} \int_0^\infty Q_0'(y) [\phi_{n0}(p') - \phi_{n0}(p)] dp' = E_{n0} \phi_{n0}(p), \quad (12)$$

where $Q_0'(y) = 1/(1-y^2)$. As mentioned before, ϕ is expanded in basis functions, followed by integrating Eq. (12) over p to generate a matrix equation. The basis functions used in previous publications [3,5] are

$$g_i^A(p) = \exp\left[\frac{-p^2 i^2}{M}\right] \quad (13)$$

and

$$g_i^B(p) = \frac{1}{(i/M)^2 + p^4}, \quad (14)$$

respectively, where M is the maximum number of basis functions used. M has a maximum because the code crashes when too many basis functions are used. The basis functions $g_i^A(p)$ and $g_i^B(p)$ have $M = 18$.

The singularity of the kernel is a major challenge in solving the integral equation with a linear potential. It was shown [3] that a simple pole remains even after subtraction. The role of the basis functions is to make possible the evaluation of the Cauchy principal value of the subtracted integral using the Sloan method [8]. To illustrate the Sloan method, we suppose that $f(x)$ has a simple pole such that

$$f(x) = \frac{g(x)}{x} \quad (15)$$

where $g(x)$ is regular. The Cauchy principal value of the subtracted integral of $f(x)$ can be evaluated if the range of integration is symmetric. For example, the numerical integration of

$$\int_{-1}^1 \frac{g(x) - g(0)}{x} dx \quad (16)$$

yields the Cauchy principal value because the point $x=0$ is skipped when quadrature points are generated in the symmetric interval $(-1,1)$. The subtraction term has zero contribution since

$$\int_{-1}^1 \frac{1}{x} dx = 0. \quad (17)$$

The purpose of this term is to justify the existence of the Cauchy principle value and to reduce numerical errors. In order to apply the Sloan method to Eq. (12), the integration variable is transformed from p to x such that x is centered at zero and its range is symmetric.

In the case of the Coulomb potential, the kernel has a logarithmic singularity,

$$Q_0(y) = \frac{1}{2} \ln \left| \frac{y+1}{y-1} \right|, \quad (18)$$

which is completely removed by Lande subtraction [1,3] because no simple pole remains after the subtraction.

The key to the success of the basis function method is the availability of a suitable set of basis functions for a particular problem. Unfortunately there is no *a priori* reason why the same set of basis functions will work in every situation. For this reason, it may be advantageous to have a method (such as the Nystrom method) that does not depend on the choice of the basis functions.

III. NYSTROM METHOD

In general, an integral equation of the Fredholm type

$$G(p)\phi(p) + \int_0^\infty F(p,p')\phi(p')dp' = \lambda\phi(p) \quad (19)$$

can be rewritten as a matrix equation as

$$\sum_{j=1}^N K_{ij} \phi_j \equiv \sum_{j=1}^N (G_{ii} + F_{ij}) \phi_j = \lambda \phi_i, \quad (20)$$

where K_{ij} is the kernel and i and j are now indices corresponding to p and p' . Instead of integrating over p from 0 to ∞ , we integrate over x from -1 to 1. Transform x_i to p_i by the transformation

$$p(x) = \tan\left(\frac{1+x}{4}\pi\right). \quad (21)$$

The mesh points x_i and the weights wt_i are generated by the gaussian quadrature rule using the routine `gauleg` from *Numerical Recipes* [7]. In order to integrate along $x \in [-1, 1]$ instead of $p \in [0, \infty)$, Eq. (19) is transformed as

$$G(x) \phi(x) + \int_{-1}^1 F(x, x') \phi(x') \frac{dp'}{dx'} dx' = \lambda \phi(x) \quad (22)$$

Changing the dummy variable inside the integral and substituting the differentiation of Eq. (21) with

$$dp = \frac{\pi}{4} \sec^2\left(\frac{1+x}{4}\pi\right) dx = \frac{\pi}{4} (1+p^2) dx \quad (23)$$

gives

$$\begin{aligned} \frac{p_i^2}{2\mu} \phi_i + \frac{\lambda_L}{4p_i^2} \int_{-1}^1 Q'_0(y \neq 1) [\phi_j - \phi_i] \sec^2\left(\frac{1+x_j}{4}\pi\right) dx_j \\ = E \phi_i. \end{aligned} \quad (24)$$

Equation (24) can now be written as a matrix equation,

$$\begin{aligned} \frac{p_i^2}{2\mu} \phi_i + \frac{\lambda_L}{4p_i^2} \\ \times \sum_{j=1}^N Q'_0(y \neq 1) \phi_j \sec^2\left(\frac{1+x_j}{4}\pi\right) wt_j, \\ - \frac{\lambda_L}{4p_i^2} \phi_i \sum_{k=1}^N Q'_0(y \neq 1) \sec^2\left(\frac{1+x_k}{4}\pi\right) wt_k = E \phi_i. \end{aligned} \quad (25)$$

The left-hand side of Eq. [25] is the kernel times the eigenvector and the right-hand side is the eigenvalue times the eigenvector. The sum over k is independent of the eigenvector, which is just a scalar. The terms on the left that have only one index i belong to the diagonal elements K_{ii} . The terms with mixed indices i and j make up the off-diagonal elements K_{ij} . More explicitly, the matrix elements of the kernel are

$$K_{ii} = \frac{p_i^2}{2\mu} - \frac{\lambda_L}{4p_i^2} \sum_k Q'_0(y \neq 1) (1+p_k^2) wt_k, \quad (26)$$

$$K_{ij} = \frac{\lambda_L}{4p_i^2} Q'_0(y) (1+p_j^2) wt_j, \quad (i \neq j). \quad (27)$$

So far the kernel \mathbf{K} is asymmetric under the interchange of i and j . We can improve the stability and the efficiency of the numerical solutions by symmetrizing Eq. (25). We do so by multiplying the equation with $p_i^2(1+p_i^2)$. It will change the original matrix equation

$$\mathbf{K} \cdot \mathbf{x} = \lambda \mathbf{x} \quad (28)$$

to an equivalent matrix equation

$$\mathbf{K}' \cdot \mathbf{x} = \lambda \mathbf{C} \cdot \mathbf{x}, \quad (29)$$

where \mathbf{C} is a diagonal matrix and $\mathbf{K}' = \mathbf{C} \cdot \mathbf{K}$. If \mathbf{C} is positive definite, meaning

$$\mathbf{x}^T \cdot \mathbf{C} \cdot \mathbf{x} \geq 0 \quad \forall \text{ vectors } \mathbf{x}, \quad (30)$$

then \mathbf{C} can be Cholesky-decomposed as

$$\mathbf{C} = \mathbf{L} \cdot \mathbf{L}^T, \quad (31)$$

where \mathbf{L} is a unique lower triangular matrix. The reason for performing Cholesky decomposition is that the new matrix

$$\mathbf{K}'' \equiv \mathbf{L}^{-1} \cdot \mathbf{K}' \cdot (\mathbf{L}^{-1})^T \quad (32)$$

is real symmetric and yields the same eigenvalues as Eq. (29). In the case of $C_{ii} = p_i^2(1+p_i^2)$, \mathbf{C} is guaranteed to be positive definite. After symmetrization, Eq. (26) does not change ($K''_{ii} = K_{ii}$) while Eq. (27) becomes

$$K''_{ij} = \frac{\lambda_L}{4p_i p_j} Q'_0(y) \sqrt{(1+p_i^2)(1+p_j^2)} wt_i wt_j \quad (i \neq j). \quad (33)$$

The eigenvalues of \mathbf{K}'' can be calculated by using standard packages such as EISPAK. In this paper, we use the `tred2` and `tqli` routines from *Numerical Recipes* [7].

IV. CORRECTION METHOD

Maung, and co-workers [3,5] have shown that the subtraction method does not completely remove the singularity at $y=1$. There is a residual simple pole term

$$- \frac{4\lambda_L}{\pi} \frac{d\phi_{n0}}{dp} \int_0^\infty \frac{p'^2}{(p'+p)^2(p'-p)} dp' \quad (34)$$

remaining after the subtraction. The basis function method evaluates the Cauchy principal value by the Sloan method as described in Sec. II. The Sloan method eliminates the simple pole term by integrating symmetrically around the singularity. Symmetrical integration involves splitting the range of integration into two intervals,

$$\int_0^\infty dp' = \int_0^{2p} dp' + \int_{2p}^\infty dp'. \quad (35)$$

The singularity at $p=p'$ is contained in the first term on the right-hand side of Eq. (35) which is assigned a symmetric transformation rule $(dp'/dx)_1$. The second term generally has a different transformation rule $(dp'/dx)_2$ because it is mapping between two different sets, namely, $(2p, \infty) \rightarrow (1, M]$ (for some real number M), such that

$$\int_0^\infty dp' \rightarrow \int_{-1}^1 \left(\frac{dp'}{dx'} \right)_1 dx' + \int_1^M \left(\frac{dp'}{dx'} \right)_2 dx'. \quad (36)$$

Notice that the division of the range of integration moves with p . If two transformation rules are used with a moving division, each row (column) of the kernel has a different way to map $[0, \infty)$ to $[-1, M]$. But the eigenvector $\phi(p)$ must be mapped to ϕ_i in a unique way. This mismatch between the mappings of the kernel and the eigenvector does not affect the basis function method (see Eq. (2.24) of Ref. [3]),

$$\sum_{i=1}^N C_i \left[\int_0^\infty \frac{p^4}{2\mu} g_j(p) g_i dp + \frac{\lambda_L}{\pi} \int_0^\infty \int_0^\infty \mathcal{Q}'_0(y) g_j(p) [g_i(p') - g_i(p)] dp' dp \right] = E \sum_{i=1}^N C_i \int_0^\infty p^2 g_j(p) g_i(p) dp \quad (37)$$

because the eigenvector C_i is an N -tuple of the coefficients of the basis function expansion of the wave function $\phi(p)$ and is independent of the transformation rules. In the case of the Nystrom method, the problem is real, at least for the range of integration that we are interested in. Therefore we cannot evaluate the Cauchy principal value by symmetric integration in the Nystrom method. In other words, a new method is needed to treat the errors arising from the simple pole term.

So far the error term Eq. (34) is not included in the Nystrom kernel in our derivation and is contributing to the errors of the eigenvalues. Since the error term [Eq. (34)] involves $d\phi/dp$, we associate it with the error of the wave function

$$\Delta\phi = \Delta p \frac{d\phi}{dp} \sim \frac{1}{N} \frac{d\phi}{dp}, \quad (38)$$

where the mesh size Δp has an N^{-1} dependence. This fact leads to an estimate of the N dependence of the error of the eigenvalue, ΔE . Let the approximate eigenvector be ϕ' and the approximate eigenvalue be E' . It is reasonable to say that an approximate kernel K acting on an approximate eigenvector ϕ' yields an approximate eigenvalue E' as in

$$K\phi' = E'\phi' \quad (39)$$

$$\Rightarrow K(\phi + \Delta\phi) = (E + \Delta E)(\phi + \Delta\phi). \quad (40)$$

It is easy to see that

$$\Delta E \approx (K - E) \frac{\Delta\phi}{\phi} = \left(\frac{K - E}{\phi} \right) \frac{d\phi}{dp} \Delta p = \epsilon \frac{1}{N}. \quad (41)$$

It is safe to assume that $(K - E)d\phi/dp \ll 1$. ϕ^{-1} can be interpreted as the normalization. The product of all of the pseudoconstants is labeled as the coefficient ϵ . The approximate eigenvalue E' produced in the background of Eq. (34) is related to the true eigenvalue E by

$$E'_n = E_n + \epsilon f_n(N), \quad (42)$$

where n is the principal quantum number, ϵ is a constant, and $f_n(N)$ is a function approximately equal to N^{-1} . In general, $f_n(N)$ varies slightly depending on the type of integral equation and the potential. As a first order approximation, assume that

$$f_n(N) = N^{-1 - \alpha(n-1)}. \quad (43)$$

The exponent of Eq. (43) is a first order Taylor series expansion of some negative unity function around $n=1$. The constant α is always taken to be small. More particularly, choose an α such that the variances of E_n , ϵ , and χ^2 are minimized in the linear fit. Finally the refinement of an eigenvalue involves generating a set of E'_n for various N by the Nystrom method and then extrapolating E_n by a χ^2 linear fit in the graph of E_n versus $f_n(N)$. In the case of Eq. (12), $\alpha = 0.004$ is an optimal choice. The numerical results are explained in Sec. VI.

The order of the Nystrom algorithm is derived from those of the `tred2` and `tqli` routines, which is $O(N^2)$ [7], compared with the basis function's $O(M^2N)$, which comes from the product of the size of the matrix M^2 and the number of integration mesh points. N is typically around 1000 and M is 20. The basis function method is generally more efficient than the Nystrom method. However, for any given set of basis functions, the accuracy of the eigenvalues cannot be improved arbitrarily by increasing the number of basis functions because M is bounded from above due to numerical errors. The prospect of improving the accuracy of the basis function algorithm depends on the availability of a set of more suitable basis functions for a specific problem. In the case of the Nystrom plus correction method, accuracy is optimized automatically by the correction scheme. The numerical results obtained by the Nystrom and basis function methods are quoted with optimal accuracy in this paper.

V. EXACT S-STATE SOLUTION

The eigenvalue of Eq. (12) can be solved exactly in configuration space. We shall use the analytic results to check our numerical results. The nonrelativistic Schrödinger equation can be written as

$$\left(\frac{d^2}{dr^2} + \frac{2}{r} \frac{d}{dr} \right) R - 2\mu[\lambda_L r - E]R = 0. \quad (44)$$

Let $S \equiv rR$, then Eq. (44) can be simplified as

$$\frac{d^2}{dr^2} S - 2\mu[\lambda_L r - E]S = 0. \quad (45)$$

TABLE I. Comparison of eigenenergies in GeV of the nonrelativistic Schrödinger equation with a linear potential between the Nystrom method and the basis Function (BF) method. The basis functions being referred to here are $g_i^B(p) = [(i/M)^2 + p^4]^{-1}$. The values of $l=0$, $\lambda_L=5$ GeV, and $\mu=0.75$ GeV are used.

n	Nystrom				BF	Exact
	$N=100$	$N=700$	$N=1400$	Corrected		
1	5.899211	5.961921	5.967339	5.972379	5.972	5.972379
2	10.268443	10.417386	10.430047	10.442010	10.443	10.442114
3	13.767781	14.054263	14.078517	14.101276	14.104	14.101524
4	16.784747	17.258395	17.297500	17.335360	17.335	17.335728
5	19.467512	20.177458	20.234722	20.291708	20.293	20.292215
6	21.891635	22.887999	22.967933	23.046820	23.053	23.047142
7	24.101339	25.435892	25.541743	25.646532	25.648	25.646268
8	26.124257	27.851711	27.986463	28.121481	27.947	28.120787
9	27.977844	30.156480	30.323418	30.493311	30.194	30.488938
10	29.672260	32.366010	32.568895	32.778297	33.340	32.769375

Define a new variable

$$x \equiv \left(\frac{2\mu}{\lambda_L^2} \right)^{1/3} [\lambda_L r - E], \quad (46)$$

such that Eq. (44) can be transformed as

$$S'' - xS = 0, \quad (47)$$

which is the Airy equation. The solution that satisfies the boundary condition $S \rightarrow 0$ as $x \rightarrow \infty$ is the Airy function $\text{Ai}(x)$. It is easy to show that the eigenenergy formula is

$$E_n = -x_n \left(\frac{\lambda_L^2}{2\mu} \right)^{1/3}, \quad (48)$$

where x_n is the n th zero of the Airy function counting from $x=0$ along $-x$. In Ref. [5], the values $\lambda_L=5$ and $\mu=0.75$ are used. In this case, the eigenenergy formula is

$$E_n = -2.554364772x_n. \quad (49)$$

VI. NUMERICAL RESULTS FOR THE S-STATE

The accuracy of the Nystrom plus correction method is sensitive to the range of N . In this paper, increments of 100 in the range of $100 \leq N \leq 1400$ are used. The reason for this choice is that there are not enough spacings between the eigenvalues for $N < 100$, and for $N > 1500$ the numerical noise begins to corrupt the monotonic convergent behavior of the eigenvalues. The correct eigenvalues are extrapolated from these numerical data by a χ^2 linear fit as described in Sec. IV. The exact S -state eigenvalues are tabulated against the numerical results obtained by the basis function method and the Nystrom plus corrections method in Table I. It shows that the numerical results obtained by the Nystrom method plus corrections are more accurate than the results obtained by the basis function method.

The kernel written for the nonrelativistic Schrödinger equation (NRSE) can be easily generalized to that of the relativistic two-body Thompson equation in the center-of-

mass frame by the replacement

$$\frac{p^2}{2\mu} \rightarrow 2(\sqrt{p^2 + m^2} - m), \quad (50)$$

where μ is the reduced mass and m is the mass of each of the two equal mass elementary particles. The numerical results obtained using the Thompson equation are compared against those using the nonrelativistic Schrödinger equation in Table II calculating to two decimal places. Our new results are exactly the same as the previous results obtained in Ref. [3] that uses basis functions $g_i^A(p)$ from Eq. (13).

VII. $l \neq 0$ KERNELS

The $l \neq 0$ kernels for the linear and Coulomb potentials contain the Legendre function of the second kind $Q_l(y)$ and its derivative, respectively. There are several mathematical issues that need to be addressed before constructing the $l \neq 0$ kernels. First of all, the definition of

$$y \equiv \frac{p^2 + p'^2}{2p'p} = \frac{1}{2} \left(\frac{p}{p'} + \frac{p'}{p} \right) \quad (51)$$

TABLE II. Comparison of the ratios of eigenenergies E_{n+1}/E_1 using the Thompson equation (TE) and the nonrelativistic Schrödinger equation (NRSE) using $l=0$ and $\lambda_L=0.2$ GeV². Mass is measured in GeV.

n	TE	NRSE	Mass
1	1.72	1.75	1.5
2	2.30	2.36	1.5
3	2.80	2.90	1.5
1	1.67	1.75	0.5
2	2.18	2.36	0.5
3	2.62	2.90	0.5
1	1.63	1.75	0.3
2	2.11	2.36	0.3
3	2.51	2.90	0.3

is easily seen to yield $y > 1$ for $p, p' > 0$. In Ref. [3], Maung *et al.* use the Legendre identity

$$Q_l(y) = P_l(y)Q_0(y) - w_{l-1}(y), \quad (52)$$

$$w_{l-1}(y) = \sum_{m=1}^l \frac{1}{m} P_{l-m}(y) P_{m-1}(y),$$

which is valid for $-1 \leq y \leq 1$ [9,10] but can be extended to $y > 1$ by analytic continuation [11]. $Q'_l(y)$ is easily obtained by straightforward differentiation. The derivative of Legendre polynomial can be calculated from one of the recurrence formulas,

$$\frac{dP_l(y)}{dy} = y \frac{dP_{l-1}(y)}{dy} + lP_{l-1}(y), \quad (53)$$

which can be computed numerically by a recursive call. The Legendre function can be generated by modifying the routine `plgndr` in *Numerical Recipes* [7] to allow $y > 1$. The accuracy of Eq. (52) and its derivatives is generally sufficient. Slightly more accurate results can be obtained by the explicit evaluation of the Neumann integral,

$$Q_l(y) = \frac{1}{2} \int_{-1}^1 \frac{1}{(y-t)} P_l(t) dt, \quad (54)$$

with derivative

$$Q'_l(y) = -\frac{1}{2} \int_{-1}^1 \frac{1}{(y-t)^2} P_l(t) dt. \quad (55)$$

The first few $Q_l(y)$ are

$$Q_0(y) = \frac{1}{2} \ln \frac{y+1}{y-1}, \quad (56)$$

$$Q_1(y) = \frac{1}{2} y \ln \frac{y+1}{y-1} - 1, \quad (57)$$

$$Q_2(y) = \frac{1}{4} (3y^2 - 1) \ln \frac{y+1}{y-1} - \frac{3}{2} y, \quad (58)$$

$$Q_3(y) = \frac{1}{4} (5y^3 - 3y) \ln \frac{y+1}{y-1} - \frac{5}{2} y^2 + \frac{2}{3}, \quad (59)$$

$$Q_4(y) = \frac{1}{16} (35y^4 - 30y^2 + 3) \ln \frac{y+1}{y-1} - \frac{35}{8} y^3 + \frac{55}{24} y, \quad (60)$$

$$Q_5(y) = \frac{1}{16} (63y^5 - 70y^3 + 15y) \ln \frac{y+1}{y-1} - \frac{63}{8} y^4 + \frac{49}{8} y^2 - \frac{8}{15}. \quad (61)$$

$Q'_l(y)$ can be obtained by the direct differentiation of $Q_l(y)$, such that

$$Q'_0(y) = \frac{1}{1-y^2}, \quad (62)$$

$$Q'_1(y) = \frac{y}{1-y^2} - \frac{1}{2} \ln \frac{y-1}{y+1}, \quad (63)$$

$$Q'_2(y) = \frac{1}{1-y^2} - \frac{3}{2} y \ln \frac{y-1}{y+1} - 3, \quad (64)$$

$$Q'_3(y) = \frac{y}{1-y^2} - \frac{15y^2-3}{4} \ln \frac{y-1}{y+1} - \frac{15}{2} y, \quad (65)$$

$$Q'_4(y) = \frac{1}{1-y^2} - \frac{35y^3-15y}{4} \ln \frac{y-1}{y+1} - \frac{35}{2} y^2 + \frac{5}{3}, \quad (66)$$

$$Q'_5(y) = \frac{y}{1-y^2} - \frac{315y^4-210y^2+15}{16} \ln \frac{y-1}{y+1} - \frac{315}{8} y^3 + \frac{105}{8} y. \quad (67)$$

As $y \rightarrow \infty$, it is easily seen that $Q_0(y) = Q'_0(y) \rightarrow 0$. This limit is true for all $Q_l(y)$ and $Q'_l(y)$ from applying the L'Hopital rule. Unfortunately straightforward numerical calculation of $Q_l(y)$ and $Q'_l(y)$ by using Eqs. (56)–(67) leads to serious numerical errors as $y \rightarrow \infty$. At the same time, it is observed that the numerical integration of Eqs. (54) and (55) are reasonably accurate in the same regime. Therefore the two representations are combined to minimize numerical error by using the Neumann integrals for $y > y_0$ and the explicit formulas for $y \leq y_0$. Our codes use $y_0 = 50$.

The subtracted momentum-space NRSE with a linear potential is given in Ref. [3], which can be simplified as

$$\begin{aligned} & \frac{p^2}{2\mu} \phi_{nl}(p) + \frac{\lambda_L}{\pi p^2} \int_0^\infty Q'_l(y) \phi_{nl}(p') dp' - \frac{\lambda_L}{\pi p^2} \phi_{nl}(p) \\ & \times \int_0^\infty Q'_0(y) dp' - \frac{\lambda_L}{\pi p} \frac{l(l+1)}{2} \phi_{nl}(p) \\ & \times \int_0^\infty \frac{Q_0}{p'} dp' + \frac{\lambda_L \pi}{p} \frac{l(l+1)}{4} \phi_{nl}(p) = E_{nl} \phi_{nl}(p). \end{aligned} \quad (68)$$

The matrix elements of a symmetric kernel for arbitrary l are

TABLE III. Eigenenergies in GeV of the nonrelativistic Schrödinger equation in momentum space (p NRSE) compared with those in the configuration space (r NRSE) and the relativistic Thompson equation in momentum space (TE). The r -space Thompson equation result is not available. The values of $n=1$, $\lambda_L=5$ GeV, and $\mu=0.75$ GeV are used.

l	p NRSE			Corrected	r NRSE Approx.
	$N=100$	$N=700$	$N=1400$		
0	5.899211	5.961921	5.967339	5.972379	5.9719
1	8.528725	8.577713	8.582413	8.586002	8.5850
2	10.823099	10.847533	10.849675	10.851526	10.8514
3	12.917124	12.904221	12.902815	12.902117	12.9020
4	14.874248	14.812422	14.805462	14.801358	14.9790
5	16.730585	16.606651	16.597636	16.586361	16.5845
TE					
0	5.859885	5.914287	5.919054	5.923117	
1	8.164379	8.202282	8.205185	8.208610	
2	10.053574	10.067261	10.068464	10.069762	
3	11.700322	11.680163	11.678063	11.676817	
4	13.185124	13.121767	13.116634	13.111239	
5	14.553134	14.437612	14.427702	14.418173	

$$\begin{aligned}
 K_{ii} = & \frac{p_i^2}{2\mu} - \frac{\lambda_L}{4p_i^2} \sum_k Q'_0(y \neq 1)(1+p_k^2)wt_k \\
 & - \frac{\lambda_L}{4p_i} \frac{l(l+1)}{2} \sum_k \frac{Q_0(y \neq 1)}{p_k} (1+p_k^2)wt_k \\
 & + \frac{\lambda_L \pi}{4p_i} l(l+1) - \frac{\lambda_L}{4p_i^2} w'_l(1)(1+p_i^2)wt_i, \quad (69)
 \end{aligned}$$

$$K_{ij} = \frac{\lambda_L}{4p_i p_j} Q'_l(y) \sqrt{(1+p_i^2)(1+p_j^2)} wt_i wt_j \quad (i \neq j). \quad (70)$$

Despite our method to control numerical noise, numerical errors still manifest themselves in the form of spurious large negative eigenvalues for $l \geq 8$. Fortunately the rest of the positive eigenvalues are accurate. Some sample eigenvalues for $0 \leq l \leq 5$ are shown in Table III, which also compares the eigenvalues generated by both the p -space and r -space codes. The r -space eigenvalues are calculated by solving NRSE using the relaxation method [13].

The Lande-subtraced momentum-space NRSE equation with a Coulomb potential is also given in Ref. [3] and is simplified as

$$\begin{aligned}
 & \frac{p^2}{2\mu} \phi_{nl}(p) + \frac{\lambda_C}{\pi p} \int_0^\infty Q_l(y) \phi_{nl}(p') p' dp' \\
 & - \frac{\lambda_C}{\pi} p \phi_{nl}(p) \int_0^\infty \frac{Q_0(y)}{p'} dp' + \frac{\lambda_C \pi}{2} p \phi_{nl}(p) \\
 & = E_{nl} \phi_{nl}(p). \quad (71)
 \end{aligned}$$

The kernel of a Coulomb potential can be symmetrized in the same way as that of a linear potential. The matrix elements are

$$\begin{aligned}
 K_{ii} = & \frac{p_i^2}{2\mu} - \frac{\lambda_C}{4} p_i \sum_k \frac{Q_0(y \neq 1)}{p_k} (1+p_k^2)wt_k + \frac{\lambda_C \pi p_i}{2} \\
 & - \frac{\lambda_C}{4} w_l(1)(1+p_i^2)wt_i, \quad (72)
 \end{aligned}$$

$$K_{ij} = \frac{\lambda_C}{4} Q_l(y) \sqrt{(1+p_i^2)(1+p_j^2)} wt_i wt_j, \quad (i \neq j). \quad (73)$$

The correction method that we have developed for the linear potential cannot be used in the Coulomb case. The only available technique of refining the eigenvalues of a Coulomb potential is by the way of increasing the number of mesh steps N . Some sample eigenvalues are shown in Table IV. Since both the linear and Coulomb potentials can be symmetrized using the same formalism, we can easily splice the two kernels together to calculate the eigenvalues of the Cornell (linear plus Coulomb) potential [12]

TABLE IV. Eigenenergies in eV of the hydrogen atom according to the nonrelativistic Schrödinger equation with $n=1$.

l	$N=100$	$N=1400$	$N=3000$	Exact
0	-25.286631	-13.600349	-13.598508	-13.598289
1	-4.579043	-3.400415	-3.399659	-3.399572
2	-1.463504	-1.511499	-1.510980	-1.510921
3	-0.634523	-0.850358	-0.849940	-0.849893
4	-0.329730	-0.544332	-0.543972	-0.543932

$$V(r) = \frac{\lambda_C}{r} + \lambda_L r. \quad (74)$$

It is not surprising that the correction method derived for the linear potential may also work for the Cornell potential because we expect that the error of the Cornell potential is dominated by the error of the linear potential term. But it is a surprise that the correction method works more accurately with the Cornell potential than the linear potential as evidenced by vanishingly small variance and χ^2 .

VIII. CONCLUSION

The basis function method requires *a priori* knowledge of the eigenfunctions in order to pick out an appropriate set of basis functions. The advantage of the Nystrom method is that no such prior knowledge of the eigenfunctions is needed. The kernel constructed by the Nystrom method is also much simpler than that by the basis function method. The eigenfunctions can be generated by the same Nystrom routines

that compute the eigenvalues. The Nystrom plus correction is more accurate than the basis function method in the cases studied in this paper. In other words, the new method has all of the advantages—elegance, accuracy, and versatility. In addition, the kernel of the relativistic and nonrelativistic equation of motion with the Coulomb and linear potential can be symmetrized in exactly the same manner. It allows the calculation of the eigenvalues of a Cornell potential readily. Since the Nystrom method can be generalized for higher l 's, we can use it to calculate the Regge trajectories. Since the Thompson equation that we have solved is a two-body equation, we can use it to analyze the experimental meson Regge trajectories [14]. This will be pursued in later work.

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