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Solving the Coulomb Schrödinger Equation in $d = 2 + 1$ via Sinc Collocation

VASILIOS G. KOURES[1]

Departments of Chemistry & Physics, Henry Eyring Building, University of Utah, Salt Lake City, Utah 84112

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We solve the light cone Coulomb Shrödinger equation in $d = 2 + 1$ via Sinc collocation. We get excellent convergence using a generalized Sinc basis set in position space. Since convergence in position space could not be obtained with more common numerical techniques, this result helps us to corroborate the conjecture that the use of a localized (square-integrable) basis set within the context of light cone quantization can yield much better convergence.

Recently, light cone quantization (LCQ) of quantum field theory has attracted considerable attention as a possible alternative method for solving non-perturbative problems in quantum field theory [1]. In this scheme, one obtains a rational, closed-form, and relativistically covariant Hamiltonian which allows one to avoid many of the severe mathematical difficulties which have plagued traditional equal time quantization techniques [1]. The discrete version of the light cone Hamiltonian allows one to model gauge theory on a computer as an eigenvalue and matrix diagonalization problem over a discrete and covariantly regularized Fock space [2].

A numerical implementation of the discretized light cone quantization (DLCQ) method to study positronium has produced promising results, but it is evident that the use of a plane wave basis will be a major bottleneck when one applies this method to more complicated models [3]. It has been suggested that the use of a localized (square-integrable) basis set would yield much better convergence for bound state computations [4, 5]. The method introduced in Ref. [5] has now been adapted to the orthogonal localized basis set of Sinc functions.

Sinc methods have increasingly been recognized as very powerful tools for attacking problems within applied physics and engineering [6, 7]. Until now, however, it was not clear how to apply Sinc methods within the context of the operator formalism of quantum field theory. This general formalism will be reported in detail elsewhere; the focus of the present paper is to demonstrate the power of the Sinc collocation method by solving the radial Coulomb equation in $d = 2 + 1$.

The motives for studying quantum electrodynamics (QED) in $2 + 1$ dimensions are numerous [8]. The lower dimensions allow a smaller number of degrees of freedom but the model still possesses independent photon degrees of freedom, unlike the $(1 + 1)$-dimensional model. The model is superrenormalizable and, when formulated with four-component spinors, it exhibits confinement [8, 9].

The non-relativistic Coulomb Schrödinger equation is derived from the LCQ formalism as follows [8]. One first derives the discretized light-cone Hamiltonian for $(2 + 1)$-dimensional QED with four-component spinors. A Tamm–Dancoff integral equation is then obtained for the "positronium" bound states. Taking the weak-coupling limit, one gets a non-relativistic integral equation which is the momentum-space Coulomb Schrödinger equation; the infrared divergences cancel between the self-mass and one-photon exchange diagrams [8]. The position-space result is then obtained by a Fourier transformation,

$$\left[-\frac{1}{m}\nabla_r^2 + \frac{g^2}{2\pi}(\gamma + \ln mr)\right]\Psi(r) = E\Psi(r), \tag{1}$$

where γ is the Euler–Mascheroni constant, m is the mass, and g is the coupling constant. It is convenient to rewrite Eq. (1) in terms of the dimensionless variables $\mathbf{x} = \frac{mg^2}{2\pi}\mathbf{r}$ and $\lambda' = (2\pi/g^2)\,E + \ln\sqrt{2g^2/m\pi}$. We get

$$(-\nabla_x^2 + \ln x + \gamma + \ln 2)\,\Psi(\mathbf{x}) = \lambda'\Psi(\mathbf{x}), \tag{2}$$

or

$$(-\nabla_x^2 + \ln x)\,\Psi(\mathbf{x}) = \lambda\Psi(\mathbf{x}), \tag{3}$$

with

$$\lambda = \lambda' - \gamma - \ln 2. \tag{4}$$

[1] E-mail: koures@dirac.chem.utah.edu.

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The separation of variables, $\Psi(\mathbf{x}) = R(x)\Theta(\theta)$, leads to $\Theta(\theta) = \exp(\pm il\theta)$, where l is the angular momentum quantum number. We are left with a radial differential equation for R which, after using the substitution [9],

$$R(x) = x^{-1/2} f(x), \tag{5}$$

transforms into a differential equation for f:

$$-f''(x) + \left[\frac{4l^2 - 1}{4x^2} + \ln x\right] f(x) = \lambda f(x). \tag{6}$$

This equation for f represents a singular Sturm–Liouville system and it can be solved by Sinc collocation [6, 7].

To this end, we begin with the definition of the Sinc function. If $a > 0$ and m is an integer, the *Sinc* function, $S(m, a)(x)$, is defined by

$$S(m, a)(x) = \frac{\sin\left[\frac{\pi}{a}(x - ma)\right]}{\frac{\pi}{a}(x - ma)}. \tag{7}$$

The theory of the Sinc series (cardinal functions) on the entire real line has been thoroughly developed. For a class of functions known as the Payley–Weiner class, the Sinc interpolation and quadrature formulas are exact [6]. However, a more practical application of Sinc approximation of functions which are in a much less restrictive class has also been developed and the absolute errors have been derived via contour integration [6]. In a nutshell, the Paley–Wiener functions are entire but a more practical class of functions should have specific growth restrictions on the real line and should be analytic only on an infinite strip centered about the real line,

$$D_S \equiv \{z \in \mathscr{C} : z = x + iy, |y| < d\}, \tag{8}$$

where $\mathscr{C}$ denotes the set of complex numbers. It turns out that the absolute error of Sinc interpolation and quadrature on such functions is exponentially damped [6].

For the problem of interest to us we need to use Sinc methods on a function f whose domain is $(0, \infty)$. The more general class just described, however, has a domain which includes the whole real line. This conflict is elegantly circumvented through the use of conformal maps [6]. For example, let ϕ be a one-to-one conformal map from some domain D to domain D_S and let ψ denote the inverse map which is also conformal. If f is analytic in D then $f \circ \psi$ is analytic in D_S. So, if a numerical process has been developed in a domain containing the whole real line, $\mathscr{R}$, then this process can be carried over to a new domain containing only a proper subset of the real line.

We will shortly see that the domain of interest to us is

$$D \equiv \left\{w \in \mathscr{C} : |\arg(\sinh(w))| < d \leq \frac{\pi}{2}\right\}. \tag{9}$$

This domain is conformally mapped onto the infinite strip D_S by the function [6]

$$z = \phi(w) = \ln(\sinh(w)). \tag{10}$$

If we let

$$w = \psi(z) = \phi^{-1}(z) = \ln(e^z + \sqrt{1 + e^{2z}}), \tag{11}$$

then

$$\Gamma \equiv \psi(\mathscr{R}) = (0, \infty), \tag{12}$$

as desired. For $a > 0$ and m an integer we define the *Sinc points*

$$x_m \equiv \psi(ma) = \ln(e^{ma} + \sqrt{1 + e^{2ma}}). \tag{13}$$

One may further verify that

$$\begin{aligned} \phi'(x_m) &= \sqrt{1 + e^{-2ma}} \\ \phi''(x_m) &= -e^{-2ma}, \end{aligned} \tag{14}$$

where the primes denote differentiation with respect to x.

Given the above definitions and maps, suppose we have a function f and that there are positive constants α, β, and C such that

$$|f(x)| \leq C \begin{cases} x^{\alpha}, & x \in (0, \ln(1 + \sqrt{2})) \\ e^{-\beta x}, & x \in [\ln(1 + \sqrt{2}), \infty) \end{cases}. \tag{15}$$

We first select a positive integer M, and then we set

$$\begin{aligned} N &= \text{ceil}\left(\frac{\alpha}{\beta} M\right) \\ a &= \sqrt{\frac{2\pi d}{\alpha M}} \leq \frac{2\pi d}{\ln(2)}, \end{aligned} \tag{16}$$

where ceil(x) rounds x to the nearest integer $\geq x$, then [6]

$$\left| f(x) - \sum_{m=-M}^{N} f(x_m) S(m, a)(\phi(x)) \right| = \mathscr{O}(\sqrt{M} \exp - \sqrt{\pi d \alpha M}), \tag{17}$$

and

$$\left|\frac{a^k}{(\phi'(x))^k}\frac{d^k}{dx^k}\left[f(x) - \sum_{m=-M}^{N} f(x_m)S(m,a)(\phi(x))\right]\right| = \mathcal{O}(\sqrt{M}\exp - \sqrt{\pi d\alpha M}). \tag{18}$$

We see that the absolute errors are exponentially damped.

The two equations (17) and (18) are all we need to solve the differential equation (6). In addition, we would like to have a normalized final answer and so we also introduce the result for Sinc quadrature [6]. Suppose we have a function F and that there are positive constants α, β, and C such that

$$|F(x)| \le C\begin{cases} x^{\alpha-1}, & x \in (0, \ln(1+\sqrt{2})) \\ e^{-\beta x}, & x \in [\ln(1+\sqrt{2}), \infty) \end{cases}. \tag{19}$$

Then [6]

$$\left|\int_0^\infty F(x)\,dx - a\sum_{m=-M}^{N}\frac{F(x_m)}{\phi'(x_m)}\right| = \mathcal{O}(\exp - \sqrt{2\pi d\alpha M}), \tag{20}$$

with M, N, and a being defined the same as before.

Now, to solve (6) we note that as $x \to 0$ the physically acceptable solution takes the form [9]

$$f \propto x^{l+1/2}. \tag{21}$$

From (15) we may thus take $\alpha = l + 1/2$. On the other hand, as $x \to \infty$ the physically acceptable solution takes the form

$$f \propto e^{-x\ln x}. \tag{22}$$

So, from (15) we may take β to be an arbitrary positive number, although, for the case $l = 0$, the choice $\beta \le 1$ works best. Next, we use (17) and (18) to approximate f and f'', respectively:

$$f(x) \approx \sum_{m=-M}^{N} S(m,a)(\phi(x))\,f(x_m) \tag{23}$$

$$f''(x) \approx \sum_{m=-M}^{N}\left\{\left[(\phi'(x))^2\frac{d^2}{d\phi^2} + \phi''(x)\frac{d}{d\phi}\right] S(m,a)(\phi(x))\right\} f(x_m). \tag{24}$$

TABLE I

First Five Eigenvalues for l Ranging from 0 to 4

	$l = 0$	$l = 1$	$l = 2$	$l = 3$	$l = 4$
λ_0	0.52643626	1.3861862	1.8443720	2.1578468	2.3962798
λ_1	1.6619365	2.0094748	2.2758614	2.4881158	2.6638815
λ_2	2.1870578	2.3943387	2.5800522	2.7390550	2.8772701
λ_3	2.5153639	2.6726676	2.8144703	2.9409664	3.0543788
λ_4	2.7677810	2.8906069	3.0049630	3.1096821	3.3373990

To evaluate these expansions at a general Sinc point x_n note that

$$\begin{aligned} S(m,a)(\phi(x))|_{x_n} &= \delta^{(0)}_{n,m} \\ \frac{d}{d\phi}S(m,a)(\phi(x))|_{x_n} &= -\frac{1}{a}\delta^{(1)}_{n,m} \\ \frac{d^2}{d\phi^2}S(m,a)(\phi(x))|_{x_n} &= \frac{1}{a^2}\delta^{(2)}_{n,m}, \end{aligned} \tag{25}$$

where $\delta^{(0)}_{n,m}$ is the Kronecker delta function and

$$\delta^{(1)}_{n,m} = \begin{cases} 0, & m = n \\ \dfrac{(-1)^{m-n}}{m-n}, & m \ne n \end{cases} \tag{26}$$

$$\delta^{(2)}_{n,m} = \begin{cases} -\dfrac{\pi^2}{3}, & m = n \\ \dfrac{2(-1)^{m-n+1}}{(m-n)^2}, & m \ne n \end{cases}. \tag{27}$$

Using these results along with (14) we may now approximate (6) via Sinc collocation,

$$\sum_{m=-M}^{N}[I^{(0)}_{n,m} + I^{(1)}_{n,m} + I^{(2)}_{n,m}]\,f(x_m) = \lambda f(x_n), \tag{28}$$

where

$$\begin{aligned} I^{(0)}_{n,m} &= \left(\frac{4l^2-1}{4x_m^2} + \ln x_m\right)\delta^{(0)}_{n,m} \\ I^{(1)}_{n,m} &= \frac{1}{a}e^{-2ma}\,\delta^{(1)}_{n,m} \\ I^{(2)}_{n,m} &= -\frac{1}{a^2}(1 + e^{-2ma})\,\delta^{(2)}_{n,m}. \end{aligned} \tag{29}$$

In the tradition of LCQ, we have formulated the problem as an eigenvalue and matrix diagonalization problem. The components of the eigenvector $f(x_m)$ can be substituted

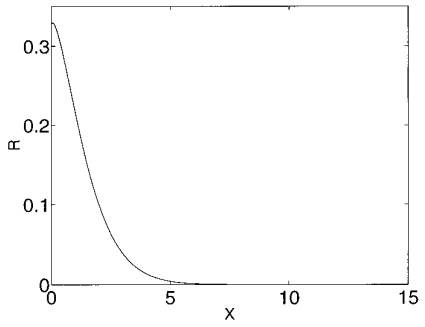

FIG. 1. Plot of normalized function $R_{0,0}(x)$ for $l = 0$ and $\lambda_0 = 0.5264$.

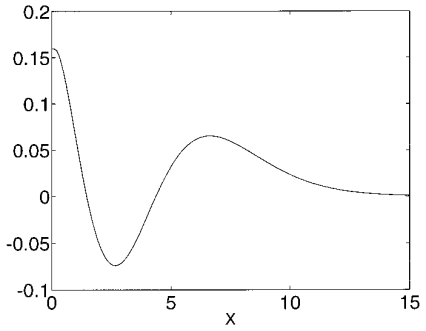

FIG. 3. Plot of normalized function $R_{2,0}(x)$ for $l = 0$ and $\lambda_2 = 2.1871$.

into (23) to compute the eigenfunction at arbitrary x. Finally, we use (5) to acquire $R(x)$ and we normalize this function by computing the norm, $\sqrt{\int_0^\infty R^2(x)\,dx}$, using the Sinc quadrature formula (20).

In Table I we list the first five eigenvalues for l ranging from 0 to 4. The diagonalization was performed with Matlab [10]. For the $l \neq 0$ values, we were able to get convergence up to five significant digits with $M = 50$, $d = \pi/4$, $\beta = 1$; the values we report here were obtained by using $M = 200$, so we see from the convergence formulas (17) and (18) that we have double precision accuracy for these values. For the $l = 0$ values, we used $M = 500$, $d = \pi/4$, and $\beta = 1/2$; again, we see from (17) and (18) that the values we report have double precision accuracy. This is a dramatic improvement over previously published position space results [9] which did not converge [8]. In Ref. [8] the first five $l = 0$ eigenvalues were computed in momentum space:

$$\begin{aligned} &\lambda_0' = 1.7969, \qquad \lambda_1' = 2.9316, \qquad \lambda_2' = 3.4475 \\ &\lambda_3' = 3.7858, \qquad \lambda_4' = 4.0380, \end{aligned} \tag{30}$$

where λ' is related to λ in Table I by (4). These momentum space results are in significant disagreement with the previously reported position space computations [9], and additional repeated attempts to get convergence in position space have failed [8]. It was concluded in Ref. [8] that "the previous position space calculation [9] was inaccurate, due to the slow, logarithmic behavior of the potential ... The momentum space calculation is much more rapidly convergent."

On the other hand, if we use (4) to convert the first column of Table I to the parameterization used in Ref. [8] we see that

$$\begin{aligned} &\lambda_0' = 1.7967991, \qquad \lambda_1' = 2.9322993, \qquad \lambda_2' = 3.4574206 \\ &\lambda_3' = 3.7857268, \qquad \lambda_4' = 4.0381439; \end{aligned} \tag{31}$$

These values are in agreement with (30) to within at least three significant digits, they converge faster, and they are more accurate (see (17) and (18)). Note further that the eigenvalues for $l \neq 0$ are actually in good agreement with the previously reported position space results [9]. (The momentum space calculations in [8] were not carried out for $l \neq 0$.) This leads us to conclude that the slow convergence of the previous position space results was not due to the slow logarithmic behavior of the potential; rather, it was due to a minor instability caused by the sign-flip of the "centrifugal" part of the potential when $l = 0$.

It is now very straightforward to use (23) along with (5) to compute any eigenfunction; these eigenfunctions are easily normalized through the use of the Sinc quadrature result (20). As a representative sample, in Figs. 1 to 3 we

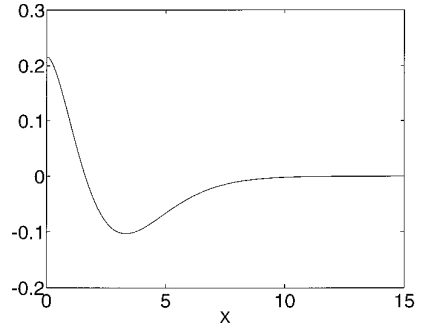

FIG. 2. Plot of normalized function $R_{1,0}(x)$ for $l = 0$ and $\lambda_1 = 1.6619$.

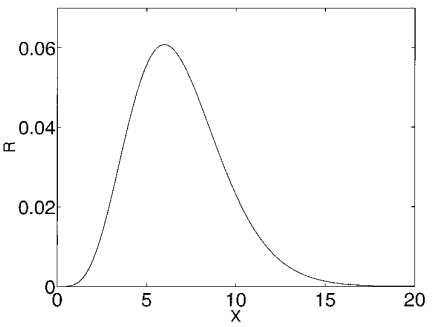

FIG. 4. Plot of normalized function $R_{0,4}(x)$ for $l = 4$ and $\lambda_0 = 2.3963$.

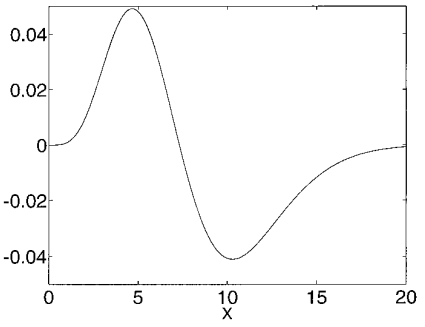

FIG. 5. Plot of normalized function $R_{1,4}(x)$ for $l = 4$ and $\lambda_1 = 2.6639$.

display the first three normalized eigenfunctions for $l = 0$; note that the number of bumps increases incrementally as we go from $n = 0$ to $n = 2$. Figures 4 to 6 show the first three normalized eigenfunctions for $l = 4$; note that the ''centrifugal'' barrier causes the bumps to move away from the center, relative to the $l = 0$ plots.

We have thus demonstrated that Sinc methods provide a very powerful tool for solving the radial Coulomb Schrödinger equation in $d = 2 + 1$. These methods are very accurate and converge very fast. This point is strongly demonstrated by the fact that convergence for the $l = 0$ values could not be attained in position space by other well-known numerical techniques. The Sinc collocation method used here may be straightforwardly extended to attack more complicated problems within quantum field theory; this formalism will be reported in detail in the future.

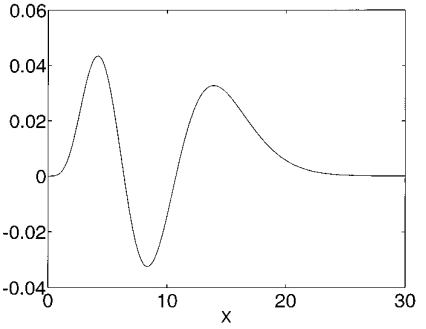

FIG. 6. Plot of normalized function $R_{2,4}(x)$ for $l = 4$ and $\lambda_2 = 2.8773$.

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