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Sinc-Integral method to solve the linear Schrodinger equation

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Abstract : The integral equation method is presented to solve the linear Schrodinger equation and obtain the eigenvalues. The eigenvalues obtained through this method are compared with Sinc-Collocation method. We show that our method is more accurate than Sinc-Collocation method. Some properties of the Sinc methods required for our subsequent development are given and utilized. Numerical examples are included to demonstrate the validity and applicability of the presented techniques.

Keywords: Linear Schrodinger equation; Sinc-Collocation method; Eigenvalue problem; Volterra integral equations; Fredholm integral equations.
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1 Introduction

In the last three decades, Sinc numerical methods have been extensively used to solve differential equations because of their exponential convergence rate[8, 9, 15, 16]. The aim of this paper is to extend the Sinc techniques to calculate the eigenvalues of Schrodinger equation on interval (a, b), within homogeneous boundary conditions $y(a)=y(b)=0$ as

$$cy''(x) + v(x)y(x) = Ey(x), \qquad \int_a^b y^2(x)dx = 1 \tag{1.1}$$

where unknown value E and function $y(x)$ are eigenvalues and eigenfunctions, respectively. Also $v(x)$ is a known function. We call $v(x)$ as potential profile. There are various methods to obtain the exact solution of the equation (1.1) [5, 6, 11]. For some potentials, the Eq (1.1) has not exact solution and it must be solved with the numerical methods such as finite difference [2, 14], variational method [3], sinc collocation and sinc galerkin [1], fixed point method [17], homotopy analysis method [4], NU method [12], etc [2, 7, 12]. In this paper we will use the sinc-integral method(SINT) i.e. we convert the equation (1.1) to an equation which contains Volterra and Fredholm integral equations and solve it with sinc collocation method. Some properties of the sinc methods required for our subsequent development are given in the next section. Formalism and Numerical examples are given in section 3 and 4 respectively.

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2 Preliminaries

In the next, a brief overview, of Sinc functions is presented. Sinc function properties are thoroughly discussed in [16]. The family of all functions f that are analytic in a domain D will be denoted by $Hol(D)$. The Sinc function is defined on the whole real line as

$$Sinc(x) = \begin{cases} \frac{sin(\pi x)}{\pi x} & x \neq 0; \\ 1 & x = 0 \end{cases} \tag{2.1}$$

For $h > 0$, the translated Sinc functions with evenly spaced nodes are given as

$$S(k,h)(x) = Sinc\left(\frac{x - kh}{h}\right) \quad k = 0, \pm 1, \pm 2, ... \tag{2.2}$$

The basis functions on (a, b) are then taken to be the composite translated Sinc functions as

$$S_k(x) = S(k,h)o\phi(x) = Sinc\left(\frac{\phi(x) - kh}{h}\right) \quad k = 0, \pm 1, \pm 2, ... \tag{2.3}$$

where $\phi : (a, b) \longrightarrow (-\infty, \infty)$ is a conformal map. Suppose the infinite strip D_d as

$$D_d = \{z \in C : |Im(z)| < d\}.$$

Then the range of ϕ^{-1} is as

$$\Gamma = \left\{\phi^{-1}(t) \in D_d : t \in (-\infty, \infty)\right\}.$$

Definition 2.1. *Let D be a simply connected domain which satisfies $(a, b) \subset D$ and α and c be positive constants. Then $L_\alpha(D)$ denotes the family of all functions $u \in Hol(D)$ which satisfies*

$$|u(z)| \leq c|Q(z)|^\alpha$$

for all $z \in D$ where $Q(z) = (z - a)(b - z)$.

The following results will be useful to obtain the discretize our system[13].

Corollary 2.2. *For $F \in L_\alpha(D_d)$, positive integer N, $h = \sqrt{\frac{\pi d}{\alpha N}}$ and $x_i = \phi^{-1}(ih)$, we have:*

$$\int_\Gamma F(x)dx \approx h \sum_{k=-N}^{N} \frac{F(x_k)}{\phi'(x_k)},$$

$$F(x) \approx \sum_{k=-N}^{N} F(x_k)S_k(x)$$

and

$$\int_a^z F(t)dt \approx h \sum_{k=-N}^{N} \delta_j^{-1}(\phi(z))\frac{F(z_k)}{\phi'(z_k)}$$

where

$$\delta_j^{-1}(z) = \frac{1}{2} + \int_0^{\frac{z}{h}-j} \frac{\sin(\pi t)}{\pi t}dt.$$

3 Formalism

The integral equation transformed from equation (1.1) is as follows

$$y(x) = Q(x)\int_a^b k_1(t, y(t))dt + f(x, y(x))\int_a^x k(x, t, y(t))dt\cdot \tag{3.1}$$

This equation is a combination of Volterra and Fredholm integral equations. In these equations, the kernels $k(x, t, y)$ and $k_1(t, y)$ are the known function and $f(x, y)$ is given. To see this, we can rewrite equation (1.1) as follows,

$$\frac{(E - v(x))y(x)}{c} = y''(x).$$

Then

$$\int_a^x \frac{(E - v(t))y(t)}{c}dt + c_1 = y'(x)\cdot$$

By putting $x = a$ we have $c_1 = y'(a)$ and so

$$\int_a^x \int_a^z \frac{(E - v(t))y(t)}{c}dtdz + xy'(a) + c_2 = y(x). \tag{3.2}$$

Now by putting $x = a$ and boundary condition $y(a) = 0$, we have $c_2 = -ay'(a)$ and then

$$\begin{aligned} y(x) &= \int_a^x \int_a^z \frac{(E - v(t))y(t)}{c}dtdz + (x - a)y'(a) \\ &= \int_a^x \int_t^x \frac{(E - v(t))y(t)}{c}dzdt + (x - a)y'(a) \\ &= \int_a^x \frac{(x - t)(E - v(t))y(t)}{c}dt + (x - a)y'(a). \end{aligned}$$

Since $y(b) = 0$, we have

$$y'(a) = -\frac{1}{b - a}\int_a^b \frac{(b - t)(E - v(t))y(t)}{c}dt$$

and so

$$y(x) = -\frac{x - a}{b - a}\int_a^b \frac{(b - t)(E - v(t))y(t)}{c}dt + \int_a^x \frac{(x - t)(E - v(t))y(t)}{c}dt\cdot \tag{3.3}$$

By letting

$$Q(x) = -\frac{x - a}{b - a},$$

$$k_1(t, y(t)) = \frac{(b - t)(E - v(t))y(t)}{c},$$

$$f(x, y(x)) = 1$$

and

$$k(x,t,y(t))=\frac{(x-t)(E-v(t))y(t)}{c},$$

we obtain relation (3.1). Equation 3.1, can be written as:

$$y(x)=E\left(Q(x)\int_a^b\frac{(b-t)y(t)}{c}dt+\int_a^x\frac{(x-t)y(t)}{c}dt\right)-Q(x)\int_a^b\frac{(b-t)v(t)y(t)}{c}dt-\int_a^x\frac{(x-t)v(t)y(t)}{c}dt. \tag{3.4}$$

Now let N be a positive integer, $h=\sqrt{\frac{\pi d}{\alpha N}}$ and $x_j=\phi^{-1}(jh)$ for $j=-N,...,N$. By the sinc collocation method, Eq. 3.4, can be written as:

$$y_j=Ea[i,j]-b[i,j] \tag{3.5}$$

where

$$a[i,j]=\left(Q(x_j)h\sum_{i=-n}^{n}\frac{b-x_i}{c\phi_i'}+h\sum_{i=-n}^{n}\frac{x-x_i}{c\phi_i'}\delta_{i-j}^{-1}\right)$$

and

$$b[i,j]=\left(Q(x_j)h\sum_{i=-n}^{n}\frac{(b-x_i)v(x_i)}{c\phi_i'}+h\sum_{i=-n}^{n}\frac{(x-x_i)v(x_i)}{c\phi_i'}\delta_{i-j}^{-1}\right).$$

Then, we can write system 3.4 as

$$Y=(EA-B)\,Y \tag{3.6}$$

where

$$A=\begin{bmatrix}\mathrm{a}_{1,1} & \cdots & \mathrm{a}_{1,2N+1}\\ \vdots & \vdots & \vdots\\ \mathrm{a}_{2N+1,1} & \cdots & \mathrm{a}_{2N+1,2N+1}\end{bmatrix}$$

$$B=\begin{bmatrix}b_{1,1} & \cdots & b_{1,2N+1}\\ \vdots & \vdots & \vdots\\ b_{2N+1,1} & \cdots & b_{2N+1,2N+1}\end{bmatrix}$$

$$Y=\begin{bmatrix}\mathrm{y}_1\\ \vdots\\ \mathrm{y}_{2N+1}\end{bmatrix}.$$

Then $\left(A^{-1}+A^{-1}B\right)Y=EY$. So, we can obtain the eigenvalues of matrix $A^{-1}+A^{-1}B$.

4 Numerical Results

In this section, we consider Eq. 1.1 through various potentials. We apply the Sinc-Integral method to all presented examples in order to obtain eigenvalues and corresponding eigenfunctions. All computations were carried out using Maple software on a personal computer.

Example 4.1. *We obtain the energy levels of equation $F''(x)=EF(x)$ on the interval $(-1,1)$ with boundary conditions $F(-1)$=$F(1)$=0. The exact eigenvalues are $E_{2n+1}=(n+1)^2\pi^2$ and $E_{2n}=\dfrac{(2n+1)^2}{4}\pi^2$.*

For numerical purpose, set $N = 20$ *and* $h = \sqrt{\frac{\pi}{N}}$. *Table (1) represents the eigenvalues obtained from sinc integral method (SINT), sinc collocation method (SC) and the exact eigenvalues. We denote the absolute errors of SINT and SC methods in eigenvalues with* $Er1 = |E_{exact} - E_{SINT}|$ *and* $Er2 = |E_{exact} - E_{SC}|$, *respectively. The error diagrams of ground state energy* (E_0) *and first excite state energy* (E_1) *are shown in figures (1) and (2), respectively.*

Table 1: Comparison of energy levels obtained through SINT and SC

Eigenvalues	SINT	SC	Exact	$Er1$	$Er2$
E_0	2.467403807	2.469915656	2.467401101	2.706×10^{-6}	2.514555×10^{-3}
E_1	9.869648165	9.879665536	9.869604404	4.3761×10^{-5}	1.0061132×10^{-1}
E_2	22.20683118	22.22924838	22.20660991	2.2127×10^{-4}	2.263847×10^{-2}
E_3	39.47911556	39.51865187	39.47841762	6.974×10^{-4}	4.023425×10^{-2}

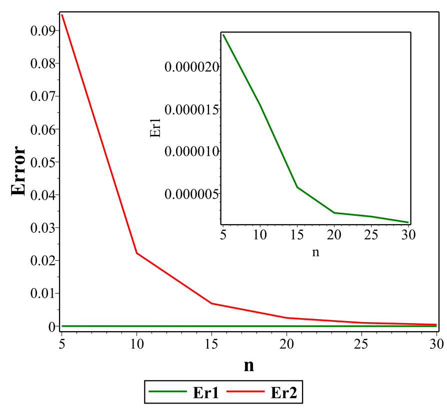

Figure 1: Error diagram of ground state energy (E_0) as a function of number of nodes

Example 4.2. *We obtain the energy levels of equation* $F''(x) + x = EF(x)$ *on the interval* $(-1, 1)$ *with boundary conditions* $F(-1){=}F(1){=}0$. *For numerical purpose, set* $N = 20$ *and* $h = \sqrt{\frac{\pi}{N}}$. *Table (1) represents the eigenvalues obtained from sinc integral method (SINT) and sinc collocation method (SC). The diagrams of ground state energy* (E_0) *and first excite state energy are* (E_1) *shown in figures (3) and (4), respectively.*

Table 2: Comparison of energy levels obtained through SINT and SC

Eigenvalues	SINT	SC
E_0	2.449871300	2.452422493
E_1	9.874861653	9.884863364
E_2	22.20995024	22.23235697
E_3	39.48102540	39.52055000

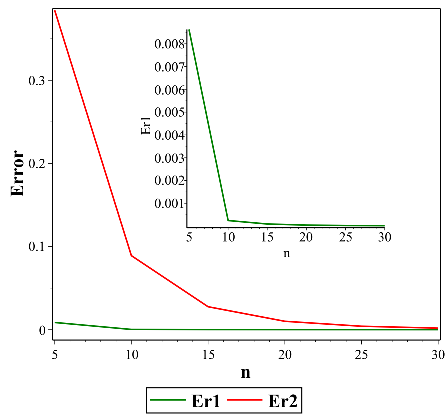

Figure 2: Error diagram of ground state energy (E_1)
as a function of number of nodes

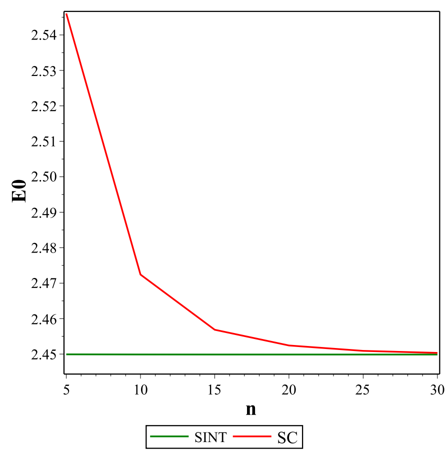

Figure 3: Diagram of ground state energy (E_0)
as a function of number of nodes

5 Conclusion

In this paper, the Sinc integral method is applied to the Schrodinger equation with homogeneous boundary conditions. The energy level obtained through Sinc integral and Sinc collocation methods are compared with each other and also with exact the solution. From the errors in the table (1), and figures (1), (2), the values of our method is more closer to the exact values. Also, from figures (3) and (4), Sinc integral method for the smaller values of n is more closer to the previous results.

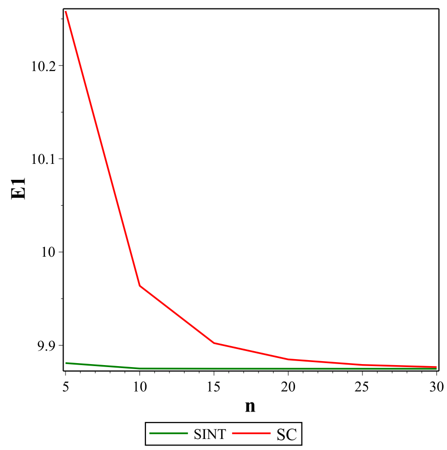

Figure 4: Diagram of ground state energy (E_1)
as a function of number of nodes

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