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Sinc-Self-consistent method to solve a class of nonlinear eigenvalue differential equation

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Abstract In this paper, we combine the sinc and self-consistent methods to solve a class of non-linear eigenvalue differential equations. Some properties of the self-consistent and sinc methods required for our subsequent development are given and employed. Numerical examples are included to demonstrate the validity and applicability of the introduced technique and a comparison is made with the existing results. The method is easy to implement and yields accurate results. We show that the sinc-self-consistent method can solve the equations on an infinite domain and produces the smallest eigenvalue with the most accuracy.

Keywords Non-linear eigenvalue differential equation · Self-consistent field iteration · Sinc method · Eigenvalues

Mathematics Subject Classification (2000) 35PX · 65LXX · 65ZXX

1 Introduction

There are some papers in which non-linear eigenvalue differential equations are studied (see [5,13]). These types of problems arise in physics, dynamic system, electronic structure calculations, etc (see [11,14,22]). In this paper, we consider the non-linear eigenvalue differential equation

$$cY''(x)+U(x)Y'(x)+V(x)Y(x)+Q(x)Y^3(x)=EY(x),\quad \int_a^b Y^2(x)dx=1 \qquad (1.1)$$

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on the interval (a,b), with homogeneous boundary conditions $Y(a)$=$Y(b)$=0, where unknown value E and function $Y(x)$ are the eigenvalues and the corresponding eigenfunctions, respectively. Also $U(x)$, $V(x)$ and $Q(x)$ are some functions. For a few well-known functions $V(x)$, the equation (1.1) has an analytical solution [3,4,6,7,18]. But most of the applied potential functions $V(x)$ have not exact solutions and they must be solved with the numerical methods. So far, different numerical methods have been used to solve Eq. 1.1 by several authors, such as variational method [1,12], fixed point method [23], homotopy analysis method [2], NU method [19], etc. However, the present paper is devoted to the numerical solution of the Eq. 1.1 by using the sinc-self-consistent (SSCF) method. To show the accuracy and robustness of the proposed schema, some examples with exact solutions are considered. This paper is organized as follows: Section 2 contains the preliminary concepts, definitions and notations of the sinc function. We present a brief overview of the self-consistent method in Section 3. Also, in Sections 4, we present the matrix form of Eq. 1.1 by the SSCF method. Section 5 is devoted to the numerical solution of some examples by the mentioned methods and compared with the finite difference self-consistent method (FDSCF). Finally, a brief conclusion is presented in Section 6.

2 Sinc method

In the last three decades, Sinc numerical methods have been extensively used to solve differential equations because of their exponential convergence rate, see e.g. [8,9,15, 20], etc. The Sinc method, which introduced and developed by F. Stenger [21], is based on the Whittaker-Shannon-Kotelnikov sampling theorem for entire functions. A brief overview of Sinc functions are presented in this section. Sinc function properties are thoroughly discussed in [17]. 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 base functions on (a,b) are then taken to be the composite translated Sinc functions as

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

We also require the derivatives of the composite translated Sinc function evaluated at the nodes x_i. The following results will be useful to obtain the discrete system[17]:

$$\delta_{ji}^{(0)} = S_j(x_i) = \begin{cases} 0 & i \neq j, \\ 1 & i = j. \end{cases} \tag{2.4}$$

$$\delta_{ji}^{(1)} = hS_j'(x_i) = \begin{cases} \frac{(-1)^{(i-j)}}{(i-j)} \; i \neq j, \\ \\ 0 \qquad i = j. \end{cases} \tag{2.5}$$

$$\delta_{ji}^{(2)} = h^2 S_j''(x_i) = \begin{cases} \frac{-2(-1)^{(i-j)}}{(i-j)^2} \; i \neq j, \\ \\ \frac{-\pi^2}{3} \qquad i = j. \end{cases} \tag{2.6}$$

$$cY''(x_j) + U(x_j)Y'(x_j) + V(x_j)Y(x_j) = EY(x_j). \tag{2.7}$$

For positive integer N, set $h = \sqrt{\frac{\pi d}{\alpha M}}$.

$$Y'(x_j) \approx \sum_{k=-N}^{N} Y_k \left(\phi' S_k'\right)(x_j) = \sum_{k=-N}^{N} Y_k \phi'(x_j)\delta_{kj}^{(1)} \tag{2.8}$$

$$\begin{aligned} Y''(x_j) &\approx \sum_{k=-N}^{N} Y_k \left(\phi'^2 S_k'' + \phi'' S_k'\right)(x_j) \\ &= \sum_{k=-N}^{N} Y_k \left(\phi'^2 \delta_{kj}^{(2)} + \phi'' \delta_{kj}^{(1)}\right)(x_j). \end{aligned} \tag{2.9}$$

3 Self-consistent field method

Let the non-linear eigenvalue problem:

$$H(X)X = \Lambda X \tag{3.1}$$

where $X \in R^{n\times 1}$, $X^T X = I$, $H(X) \in R^{n\times n}$ is a matrix that has a special structure and $\Lambda \in R$ is a diagonal matrix consisting of the smallest eigenvalues of $H(X)$. Some researches in [16,24] investigated the convergence of Self-consistent field iteration(SCF) which defined as follow to solve problem (3.1):

$$\begin{cases} \textit{Pick any initial guess} \mathrm{X}^{(0)} \\ 1.\textit{For} \text{ i = 1,2, . . . } \textit{until convergence} \\ 2.\textit{Construct } \mathrm{H}^{(i)} = H(X^{(i-1)}); \\ 3.\textit{Compute } \mathrm{X}^{(i)} \text{ such that } H^{(i)}X^{(i)} = X^{(i)}\Lambda^{(i)}, \text{ and } \Lambda^{(i)} \\ \textit{contains the smallest eigenvalues of } \mathrm{H}^{(i)}; \\ 4.\textit{End for} \end{cases} \tag{3.2}$$

Yang et al. in [24] show that for some class of problems, the SCF iteration produces a sequence of approximate solutions that contains two convergent subsequence. They used the standard distance measure [10] between two columns $X, Y \in R^{n\times k}$ i.e., if $X^T X = Y^T Y = I_k$,

$$dist(X,Y) = \|XX^T - YY^T\|_2$$

where for every matrix $A \in R^{m\times n}$,

$$\|A\|_2 = \sup_{x\neq 0} \frac{\|Ax\|_2}{\|x\|_2}.$$

They obtained the following theorem:

Theorem 3.1 *Let $X^{(0)} \in R^{n\times k}$ be the initial guess to the solution of the non-linear eigenvalue problem (3.1) that satisfies ${X^{(0)}}^T X^{(0)} = I_k$. If columns of $X^{(i)} \in R^{n\times k}$ contain eigenvectors associated with the smallest k eigenvalues of $H(X^{(i-1)})$, as we would obtain when applying the SCF iteration to (3.1), and if the gap between the kth and the $k+1$st eigenvalues of $H(X^{(i)})$ is greater than or equal to $\delta > 0$ for all i, then*

$$\lim_{i\to\infty} dist^2(X^{i+2}, X^i) = 0.$$

4 Main results

In this section, we obtain the matrix generated by the sinc method. By using the collocation method and relations (2.7), (2.8), and (2.9) we have

$$\sum_{k=-N}^{N} Y_k \left(c{\phi'}^2 \delta_{kj}^{(2)} + \left(c\phi'' + U\phi' \right) \delta_{kj}^{(1)} \right)(x_j) + V(x_j)Y_j + Q(x_j)Y_j^3 = EY_j. \quad (4.1)$$

Let

$$p_{ij} = \left(c{\phi'}^2 \delta_{kj}^{(2)} + \left(c\phi'' + U\phi' \right) \delta_{kj}^{(1)} \right)(x_j).$$

Then, we can write system (4.1) as

$$(X + QZ)\, Y = EY \quad (4.2)$$

where

$$X = \begin{pmatrix} p_{-n,-n} + v_{-n} & \cdots & p_{-n,n} \\ \vdots & \ddots & \vdots \\ p_{n,-n} & \cdots & p_{n,n} + v_n \end{pmatrix}$$

$$Q = \begin{pmatrix} q_{-n} & 0 & \cdots & 0 \\ 0 & q_{-n+1} & & 0 \\ \vdots & & \ddots & \vdots \\ 0 & 0 & & q_n \end{pmatrix}$$

$$Y = \begin{pmatrix} y_{-n} \\ \vdots \\ y_n \end{pmatrix}$$

and $Z = (DiagY)^2$. Now, we must solve the non-linear eigenvalue problem $H(Y)Y = EY$, where

$$H(Y) = X + Q(DiagY)^2.$$

For this end, let $Z^0 = 0$. We use the following algorithm to solve non-linear eigenvalue problem (4.2).
1. For $i = 1, 2, ...$ until convergence
2. Construct $H^{(i)} = X + QZ^{(i-1)}$
3. Compute $F^{(i)}$ such that $H^{(i)}F^{(i)} = E^{(i)}F^{(i)}$, and $E^{(i)}$ contains the smallest eigenvalues of $H^{(i)}$;
4. Construct $Y^{(i)}$ such that $Y^{(i)} = \frac{F^{(i)}}{\|F^{(i)}\|_2}$
5. Construct $Z^{(i)} = (DiagY^{(i)})^2$
6. End for
So, we can obtain the eigenvalues and eigenfunctions of Eq. 1.1.

5 Numerical results

In this section, we consider Eq. 1.1 through various functions $V(x)$. We denote the eigenvalues of Eq. 1.1 with E_i. Moreover, we report the CPU time for our method. All computations were carried out using Maple software on a personal computer. The computer processing properties are as follows: Intel(R) Core(TIM) i7-6500U CPU@GHz 2.59GHz, RAM: 8.00 GB.

Example 5.1 We first consider Eq. 1.1 on $(-\infty, +\infty)$ with $c = -\frac{1}{2}$, $U(x) = 0$ and $V(x) = \frac{1}{2}x^2$. In [12], the even eigenvalues are obtained by the variational method as

$$E_n = -cb^2 - c(n + \frac{1}{2})(a^2 - \frac{1}{2ca^2}) + \frac{Qa}{h_n^2} I_n. \tag{5.1}$$

Where $h_n = 2^n\sqrt{\pi}n!$, $I_n = \int_{-\infty}^{\infty} H_n^4(x)e^{-2x^2}dx$, $H_n(x)$ are Hermit polynomials [4], a is a positive root of

$$\frac{1}{2c} = -a^4 + \frac{QI_n}{2c(2n+1)h_n^2}a^3,$$

and the wave functions are in the form $Y_n(x) = \sqrt{\frac{a}{h_n}}H_n(ax)e^{-\frac{a^2x^2}{2}}$. In this example, we set $Q = 1$, $N = 30$ and $h = \sqrt{\frac{\pi}{N}}$. Let $i = 10$ be the number of iterations. Table 5.1 represents the even eigenvalues obtained from SSCF and results of reference [12]. In figure (5.1), we show the convergence of this method through variation of smallest eigenvalue as a function of the number of iterations for $Q = 1, 2, 3$. We observe that the convergence of our method is better full-filled when the non-linear parameter $|Q|$ has smaller values. Also, figure (5.2), shows the variation of the minimum eigenvalue as a function of Q. This figure shows that the method works better, for smaller values of the non-linear coefficient $|Q|$.

Table 5.1 Comparison of the eigenvalue of the example 5.1 obtained through SSCF and Ref [12] .

Eigenvalues	SSCF	Ref [12]
E_0	0.8699440500	0.8726179080
E_2	2.652621066	2.753164076
E_4	4.610725009	4.709682021
E_6	6.591042186	6.685128136
CPU time(s)	36.9	–

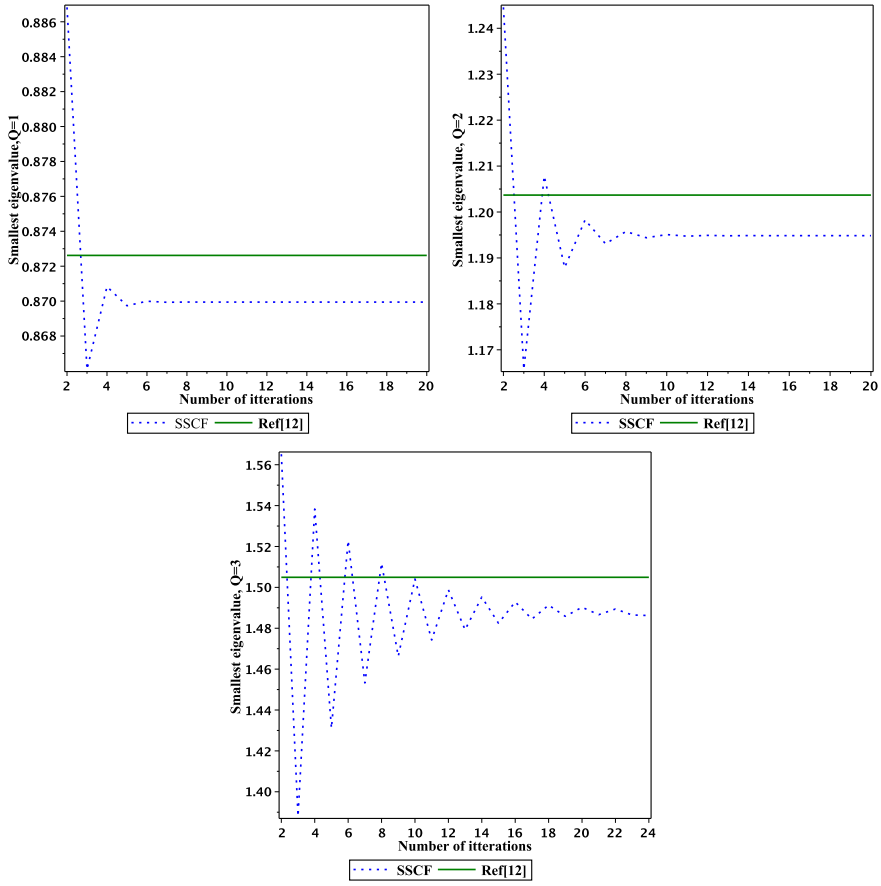

Fig. 5.1 Panels show the variations of the smallest eigenvalues as a function of the number of iterations for $Q = 1,2,3$ (example 5.1).

Example 5.2 Consider Eq. 1.1 on $(-1,1)$ with $c{=}-\frac{1}{2}$, $Q(x) = Q \leq 0$ and $U(x) = V(x) = 0$. By [7], we obtain the solution of this equation in the form

$$Y(x) = C.cn(\lambda(x-x_0),k)$$

where, λ and x_0 are arbitrary constants and k and C are determined as follows:

$$k^2 = \frac{\lambda^2 - 2E}{2\lambda^2}, \quad C^2 = -\frac{\lambda^2 - 2E}{2Q}$$

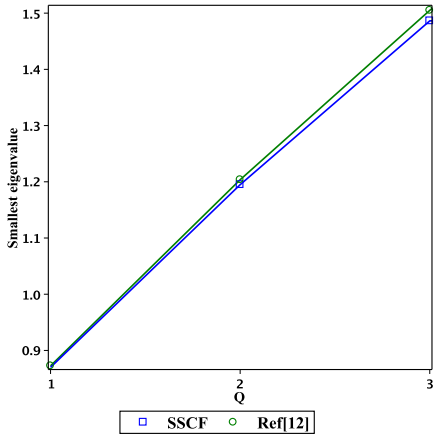

Fig. 5.2 Variation of the smallest eigenvalue as a function of Q(example 5.1).

and then

$$k = \frac{C\sqrt{-Q}}{\lambda}, \quad C^2 = -\frac{\lambda^2 - 2E}{2Q}.$$

Since for odd functions $Y(0) = 0$ and for even functions $Y'(0) = 0$, we have $x_0 = 0$ and $x_0 = 3EllipticK(k)$, respectively. By using the constants x_0, even and odd solutions of equations can be obtained

$$Y_{even} = Ccn(\lambda x, k), \qquad Y_{odd} = C\sqrt{1-k^2}\frac{sn(\lambda x, k)}{dn(\lambda x, k)}.$$

Now by using $Y(\pm 1) = 0$ and $\int_{-1}^{1} Y^2 = 1$, we have

$$E_n = \frac{(1-2k^2)(EllipticK(k))^2 n^2}{2}$$

where n is the number of eigenvalues and k is the solution of the equation

$$-\frac{2EllipticK(k)}{Q}(EllipticE(k) - (1-k^2)EllipticK(k)) = \frac{1}{n^2}.$$

Let $N = 100$ be the number of nods and $i = 10$ be the number of iterations. Table (5.2), presents the eigenvalues obtained by SSCF, FDSCF and the exact values for $Q = -1$ as well as the absolute errors of SSCF and FDSCF methods with $Er_S = |E_{Exact} - E_{SSCF}|$ and $Er_F = |E_{Exact} - E_{FDSCF}|$, respectively. In figure (5.3), we show the convergence of SSCF and FDSCF methods through variation of the smallest eigenvalue and error as a function of the number of nodes for $Q = -1$. Also, figure (5.4) shows the convergence of SSCF and FDSCF methods through variation of the error as a function of the number of eigenvalues for $Q = -1$. This figure shows that the FDSCF works better for the seven lowest eigenvalues. However, the error is fixed for all obtained eigenvalues. Therefore, when the few lowest eigenvalues are required,

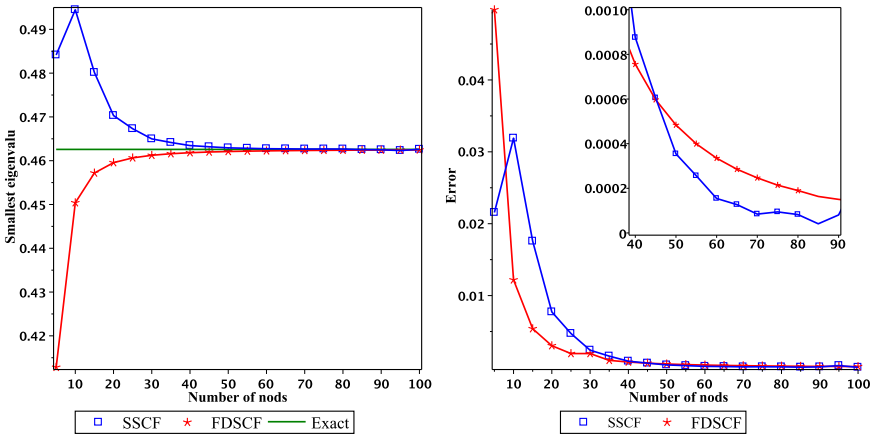

Fig. 5.3 the left figure shows the variation of the smallest eigenvalue as a function of the number of nods and the right figure shows the variation of the error as a function of the number of nods for $Q = -1$ (example 5.2).

both of the presented methods can be used. But if we need the whole eigenvalue spectrum or at least a large portion of the eigenvalues, the SSCF is more reliable because we can more generally know the errors of higher index eigenvalues. Figure (5.5), also shows the variation of the smallest eigenvalue and the error of SSCF and FDSCF as a function of Q. This figure shows that the method works better, for smaller values of the non-linear coefficient $|Q|$. We observe that the error of our method is smaller when the non-linear parameter $|Q|$ has smaller values. However, this is true for smaller eigenvalues. Also, we see that for larger eigenvalues, we have not a rule of thumb for larger value of the eigenvalues.

Table 5.2 Comparison of the exact eigenvalues of example 5.2 obtained through SSCF and FDSCF, for $Q = -1$.

Eigenvalues	SSCF	FDSCF	Exact	Er_S	Er_F
E_0	0.4626016170	0.462459047	0.462579418	2.21990e-05	1.20371e-04
E_1	4.443995283	4.442553417	4.179929550	0.264065733	0.262623867
E_2	10.60665214	10.59860958	10.35117007	0.25548207	0.24743951
E_3	19.24142796	19.21512218	18.98801387	0.25341409	0.22710831
E_4	30.34402278	30.28031329	30.091750	0.25227278	0.18856329
E_5	43.91437108	43.78267728	43.662690	0.25168108	0.11998728
E_6	59.95245468	59.70867902	59.70093840	0.25151628	0.00774062
E_7	78.45806592	78.04253889	78.20653790	0.25152802	0.16399901
CPU time(s)	161	113	–	–	–

Example 5.3 Consider Eq. 1.1 on $(-1,1)$ with $c{=}-1$, $U(x) = 0$ and $V(x) = 0.452\cos(\pi(1-x))$. In [1], the eigenvalues are obtained by using the discretized Euler-Lagrange variational method. Let $N = 100$ and $i = 10$. Table (5.3) represents the smallest eigenvalue obtained from reference [1] as well as SSCF and FDSCF methods for $Q(x) = 0.5...2$.

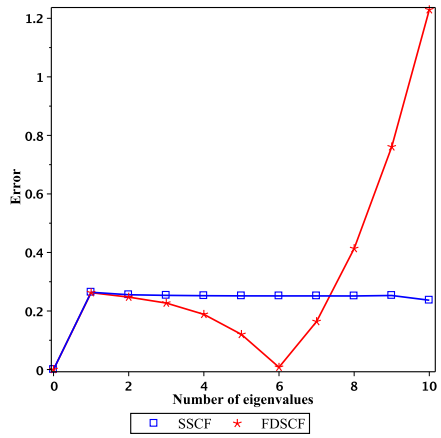

Fig. 5.4 Variation of the error as a function of the number of eigenvalues for $Q = -1$ (example 5.2).

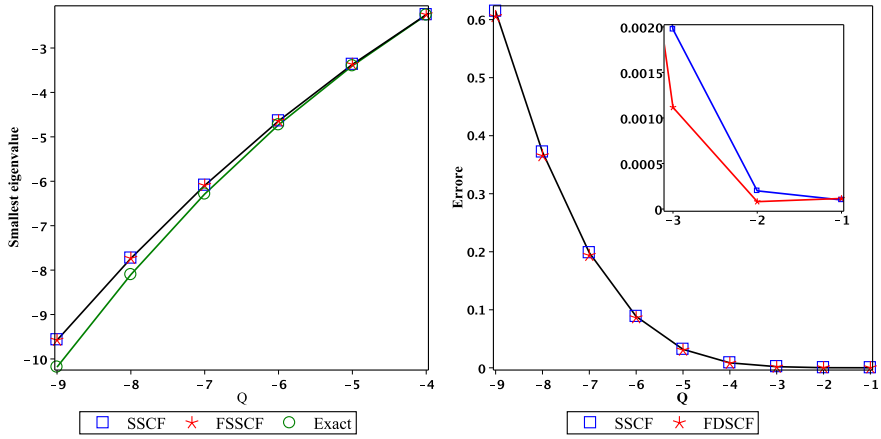

Fig. 5.5 The left figure shows the variation of the smallest eigenvalue as a function of Q and the right figure shows the variation of the error as a function of Q(example 5.2).

This table shows that both of the methods work well in this situation. However, the CPU time of the SSCF is greater than the FDSCF method. In figure (5.6), we show the variation of the smallest eigenvalue as a function of Q. Again, we see that both of the presented methods excellently work in this example.

6 Conclusion

In this paper, the SSCF method is applied to a class of non-linear eigenvalue differential equation with homogeneous boundary conditions. The eigenvalues obtained through this method are compared with exact values and some other references. To demonstrate the efficiency and effectiveness of the proposed method, three examples

Table 5.3 Comparison of the smallest eigenvalue of example 5.3 obtained through SSCF, FDSCF and Ref [1].

Q	SSCF	FDSCF	Ref [1]	CPU time$_{SSCF}$	CPU time$_{FDSCF}$
0.5	2.616897689	2.616948710	2.616951848	172	108
1	2.990597503	2.990592936	2.99059549	172	106
1.5	3.360892363	3.359893114	3.35989571	172	112
2	3.726258011	3.725158240	3.725158948	174	109

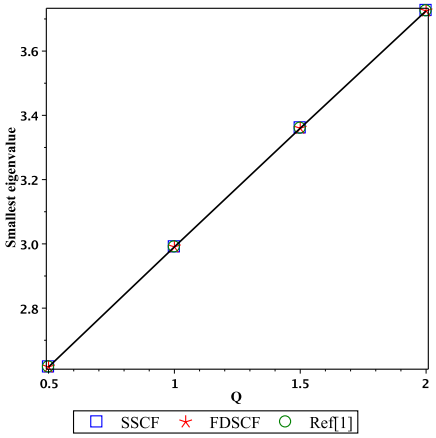

Fig. 5.6 Variation of the smallest eigenvalue as a function of the number of Q (example 5.3).

are examined. Based on the numerical experiments, we conclude the method works better, for smaller values of the non-linear coefficient $|Q|$ in equation 1.1. Also, we see that the results for the smallest eigenvalue have the best accuracies. But accuracy is lesser satisfactory for larger eigenvalues. We see, the CPU time of the SSCF is greater than the FDSCF method but the SSCF is more reliable because we can more generally know the errors of higher index eigenvalues. However, the difference in the CPU time is not so large that we are not able to solve realistic physics and engineering problems.

Declaration of interests

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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