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Construction of self-similar shape invariant potentials with the Padé approximation

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Abstract

We study here the self-similar shape invariant potential (SSSIP) proposed by Barclay *et al* (1993 *Phys. Rev.* A **48** 2786) in the context of supersymmetric quantum mechanics. The superpotential of SSSIP, $W(x)$, obeys an ordinary differential equation involving W and its derivative at two different spatial points, and hence cannot be solved with standard numerical methods. In addition, Taylor series expansion of $W(x)$ about $x = 0$ also diverges at large x. To provide an effective numerical scheme to construct the superpotential, we use the Padé approximation to express $W(x)$ as a fraction of polynomials in x. We find that the homogeneous two-point Padé approximant can indeed yield accurate values of the superpotential for all x.

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1. Introduction

The study of supersymmetric quantum mechanics (SQM) bloomed in the early 1980s as a fruitful byproduct of the investigation of the breakdown of supersymmetry (SUSY) in quantum field theory (see, e.g., [1–6] and references therein). The basic idea of SQM is simple and analogous to that of the factorization method proposed in the mid-twentieth century [7–9]. However, SQM has been shown to be a systematic method to understand why certain potentials, termed as shape invariant potentials (SIPs), are exactly solvable, and to generate new exactly solvable potentials [10–12]. More surprisingly, the theory of SQM is also adapted to descriptions of other physical phenomena such as inverse scattering and solitons [13–18].

The major concern of the present paper is a special kind of SIP, namely self-similar SIP (SSSIP). SSSIP was first considered in the context of SQM by Barclay *et al* [11]. The physical significance of SSSIPs is that they are reflectionless potentials supporting an infinite number of bound states. It is well known that reflectionless potentials of the Schrödinger equation can lead to multi-soliton solutions of the Korteweg-de Vries (KdV) equation (see,

e.g., [13–18]). In particular, the number of bound states of the potential correspond to the number of solitons. Like other SIPs, the spectrum of SSSIPs can be found exactly. However, to our knowledge, there is no closed form analytic solution to its superpotential $W(x)$, which obeys an ordinary differential equation involving W and its derivative at two different spatial points. Such a finite-difference ordinary differential equation is not amenable to standard numerical methods in the absence of other theoretical input. Instead, Barclay *et al* have developed a power series about $x = 0$ to supplement the differential equation and succeeded in obtaining the superpotential and the associated potential as well [11]. However, they have also shown that the power series diverges for x greater than a certain value.

The aim of our study here is to obtain an approximate analytic expansion for the superpotential of SSSIPs, which can yield accurate numerical results for all values of x. The tool we used is the standard Padé approximation (see, e.g., [19]). First of all, we construct a one-point homogeneous Padé approximant from the power series about $x = 0$. We find that this one-point homogeneous Padé approximant can readily reproduce the superpotential for a large range of x, thus extending the validity of the original power series about $x = 0$ beyond its radius of convergence. However, the one-point Padé approximant fails to yield the correct asymptotic value of the superpotential at large x. We therefore further make use the two-point homogeneous Padé approximant, which is able to capture the essence of the superpotential at both small and large x, to approximate the superpotential. We find that the result obtained from the two-point homogeneous Padé approximant is in fact accurate everywhere. In addition, we are also able to fix an unknown constant in the power series expansion of $W(x)$ developed about the point $x = \infty$ [11]. The Padé approximant developed here for the superpotential of SSSIPs can be used to generate the associated potential and in turn the solution of the KdV equation which describes the evolution of an infinite number of solitons.

The structure of this paper is as follows. To make our paper a self-contained one, we briefly review the basic idea of SQM and SIPs, and introduce the property of SSSIPs in sections 2 and 3, respectively. We then apply the one-point Padé approximant to approximate the superpotential and discuss the effect of the center of the approximant on the accuracy of the approximation in section 4. In section 5 we extend our study using the two-point Padé approximant and show that it outperforms the one-point Padé approximant. We end our paper with a discussion in section 6.

2. SQM and SIPs

As in the factorization method [7–9], the fundamental principle of SQM is to express a given Hamiltonian $\hat{H}_1$ (in units of $2m = \hbar = 1$) as the product of two operators $\hat{A}$ and $\hat{A}^\dagger$:

$$\hat{H}_1 \equiv -\frac{\mathrm{d}^2}{\mathrm{d}x^2} + V_1(x) = \hat{A}^\dagger \hat{A}, \tag{2.1}$$

where the two operators $\hat{A}$ and $\hat{A}^\dagger$ are expressible in terms of a superpotential $W(x)$:

$$\hat{A} = \frac{\mathrm{d}}{\mathrm{d}x} + W(x), \tag{2.2}$$

$$\hat{A}^\dagger = -\frac{\mathrm{d}}{\mathrm{d}x} + W(x). \tag{2.3}$$

Following directly from (2.1), it is obvious that $W(x)$ satisfies the equation

$$V_1(x) = W^2(x) - W'(x). \tag{2.4}$$

Hereafter, we use a prime to denote differentiation with respect to x.

The supersymmetric partner Hamiltonian of $\hat{H}_1$, $\hat{H}_2$, is defined by

$$\hat{H}_2 \equiv -\frac{\mathrm{d}^2}{\mathrm{d}x^2} + V_2(x) = \hat{A}\hat{A}^\dagger, \tag{2.5}$$

where

$$V_2(x) = W^2(x) + W'(x). \tag{2.6}$$

The energy spectra of these two supersymmetric partner Hamiltonians, denoted as $E_0^{(i)} < E_1^{(i)} < E_2^{(i)} < \cdots$ ($i = 1, 2$ for the spectra of $\hat{H}_1$ and $\hat{H}_2$, respectively), are closely related to each other. For unbroken SUSY where $E_0^{(1)} = 0$ and $\hat{A}\psi_0^{(1)} = 0$, with $\psi_0^{(1)}$ being the ground state wavefunction of $\hat{H}_1$, the two spectra are almost identical in the sense that

$$E_{n+1}^{(1)} = E_n^{(2)}. \tag{2.7}$$

Furthermore, for SIPs satisfying the shape invariant relation:

$$V_2(x; a_1) = V_1(x; a_2) + R(a_1), \tag{2.8}$$

where a_1 and $a_2 = f(a_1)$ are free parameters characterizing the partner potentials V_1 and V_2, respectively, f and R are functions of a_1, the entire spectrum of $\hat{H}_1$ can be readily generated:

$$E_0^{(1)} = 0, \qquad E_n^{(1)} = \sum_{k=1}^{n} R(a_k) \qquad \text{for} \quad n \geqslant 1, \tag{2.9}$$

with $a_k = f^{k-1}(a_1)$. More interestingly, many exactly solvable potentials, including the three-dimensional oscillator potential, the Coulomb potential, the Morse potential and the Eckart potential, are SIPs (see, e.g., [4, 6, 20]). SIPs can be categorized according to the nature of the function $f(a_1)$ (see, e.g., [6]). If $f(a_1) = a_1 + \alpha$, where α is an arbitrary constant, the family of SIPs are said to be related by translation, termed as translational SIPs (TSIPs). On the other hand, if

$$f(a_1) = qa_1, \tag{2.10}$$

with q being a scaling parameter, such SIPs are said to be related by scaling and called scaling SIPs (SSIPs) [11, 12]. Another kind of SIP discovered more recently is the cyclic shape invariant potential (CSIP) [21–23]. For CSIPs, the parameters a_1 and a_2 are related by a cyclic function f of period-p, such that

$$a_{p+1} = f^p(a_1) = a_1, \tag{2.11}$$

with p being a positive integer. The superpotentials of all TSIPs can be expressed in closed analytic forms, whereas analytic forms of the superpotentials of SSIPs and CSIPs (except for the period-2 CSIP [21]) are not available to our knowledge.

3. Self-similar potentials

The concept of self-similar potentials (SSP) was first discussed by Shabat [24] and Spiridonov [25] in the context of inverse scattering and q-deformation of the single-soliton solution of the Rosen–Morse potential. Superpotentials are termed as self-similar if

$$W_{i+1}(x) = pW_i(px), \tag{3.1}$$

where $i = 1, 2, \ldots, 0 < p < 1$ is a deformation parameter, and $W_i(x)$ is the ith superpotential in a sequence of SIPs. Subsequent to the investigation of Shabat [24] and Spiridonov [25], Barclay *et al* discovered that SSPs are in fact a special kind of SSIP [11]. To reveal relevant properties of SSPs, we sketch here the argument of Barclay *et al* [11].

First of all, the superpotential $W(x, a_1) \equiv W_1(x)$ and $R(a_1)$ of a SSIP in (2.8) are expanded in terms of series of the parameter a_1:

$$W(x, a_1) = \sum_{j=0}^{\infty} g_j(x) a_1^j, \tag{3.2}$$

$$R(a_1) = \sum_{j=0}^{\infty} R_j a_1^j, \tag{3.3}$$

where $g_j(x)$ are the functions of x only, and R_j are constants. Using these expansions, together with (2.4), (2.6), (2.8) and (2.10), it is straightforward to show that

$$2g_0'(x) = R_0, \tag{3.4}$$

$$g_1'(x) + 2d_1 g_0(x) g_1(x) = r_1 d_1, \tag{3.5}$$

$$g_n'(x) + 2d_n g_0(x) g_n(x) = r_n d_n - d_n \sum_{j=1}^{n-1} g_j(x) g_{n-j}(x), \qquad n = 2, 3, \ldots, \tag{3.6}$$

where

$$r_n = \frac{R_n}{(1-q^n)}, \qquad d_n = \frac{(1-q^n)}{(1+q^n)} \tag{3.7}$$

for $n = 1, 2, 3, \ldots$. In the simplest case with $g_0 = 0$ and $R_0 = 0$, equations (3.4)–(3.6) can be integrated in succession, yielding

$$g_1(x) = r_1 d_1 x, \tag{3.8}$$

$$g_n(x) = d_n \int \left(r_n - \sum_{j=1}^{n-1} g_j(x) g_{n-j}(x) \right) \mathrm{d}x, \tag{3.9}$$

and the superpotential W can be readily obtained by putting these results into (3.2).

Barclay *et al* [11] further considered a special kind of SSIP satisfying the condition

$$R_n = 0 \tag{3.10}$$

for all $n \geqslant 2$. The series expansion of the superpotential is particularly simple:

$$W(x, a_1) = \sqrt{a_1} \sum_{i=1}^{\infty} \beta_i (\sqrt{a_1} x)^{2i-1}, \tag{3.11}$$

where $\beta_1 = d_1 r_1 = R_1/(1+q)$, and for $n = 2, 3, \ldots$

$$\beta_n = -\frac{d_n}{2n-1} \sum_{j=1}^{n-1} \beta_j \beta_{n-j}. \tag{3.12}$$

Such a kind of superpotential is characterized by the function $F(x)$ defined by

$$F(x) = W(x, a_1 = 1) = \sum_{i=1}^{\infty} \beta_i x^{2i-1}, \tag{3.13}$$

and hence

$$W(x, a_1) = \sqrt{a_1} F(\sqrt{a_1} x). \tag{3.14}$$

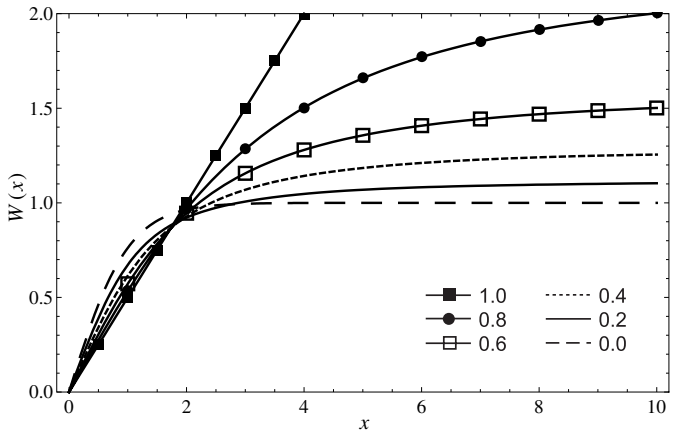

Figure 1. The exact superpotential $W(x)$ of SSSIPs is plotted against x for different values of the scaling constant q, namely, $q = 1.0$ (solid line with filled squares), 0.8 (solid line with filled circles), 0.6 (solid line with empty squares), 0.4 (short dashed line), 0.2 (solid line) and 0.0 (long dashed line), respectively.

It is easy to see that this particular kind of SSIP, which satisfies $W_{i+1}(x) = W_1(x, q^i a_1)$ and (3.14), obeys (3.1) as well, and is indeed self-similar with the deformation parameter given by $p = \sqrt{q}$. Therefore, we term it as self-similar SIP (SSSIP) in the present paper.

According to (3.11) and (3.12), the superpotential of a SSSIP can be expanded as a power series in x:

$$W(x) = \frac{C_1}{1+q}x - \frac{1}{3}\left(\frac{C_1}{1+q}\right)^2 \frac{1-q^2}{1+q^2}x^3 + \cdots, \tag{3.15}$$

with $C_1 = R_1 a_1$, and hereafter its dependence on a_1 is suppressed. Higher-order expansion can be obtained in a systematic way. However, the radius of convergence R_c of the series in (3.15) is shown to be finite, satisfying the following inequalities [11]:

$$\frac{\pi}{2} \leqslant \sqrt{C_1} R_c \leqslant \frac{\pi}{2}\sqrt{\frac{1+q}{1-q}}. \tag{3.16}$$

Therefore, it is impossible to generate the superpotential $W(x)$ with (3.15) for x greater than R_c. To solve this $W(x)$ for all $x \in [0, \infty)$, Barclay *et al* have suggested the following recipe [11]. First, one can use the shape invariant condition in (2.8) to find a finite-difference differential equation:

$$W^2(x) + W'(x) = q\,W^2(\sqrt{q}x) - \sqrt{q}\frac{\mathrm{d}W(\sqrt{q}x)}{\mathrm{d}x} + C_1. \tag{3.17}$$

Second, one can supplement this equation with the expansion (3.15), which can yield accurate result for sufficiently small x. With the input of the value of $W(\sqrt{q}x)$ generated from (3.15) at a small $\sqrt{q}x$, equation (3.17) can be solved for a larger domain of x. Hence, by repeatedly substituting the value of $W(x)$ obtained from the previous round of calculation into the rhs of (3.17), $W(x)$ can be evaluated for all x. Figure 1 shows the superpotential obtained through this numerical scheme for SSSIPs with $q = 0, 0.2, 0.4, 0.6, 0.8, 1.0$. It is interesting to note that SSSIPs with $q = 1$ and $q = 0$, respectively, correspond to the one-dimensional simple harmonic potential ($W(x) \propto x$) and the Rosen–Morse potential ($W(x) \propto \tanh\sqrt{C_1}x$) [11], and these two limiting cases of the superpotential are clearly shown in figure 1.

The asymptotic behavior of $W(x)$ as $x \to \infty$ can also be derived from the finite-difference differential equation in (3.17), which can be recast into the following form:

$$W_\infty^2(y) - y^2 \frac{\mathrm{d}W_\infty(y)}{\mathrm{d}y} = q W_\infty^2(y/\sqrt{q}) + \sqrt{q} y^2 \frac{\mathrm{d}W_\infty(y/\sqrt{q})}{\mathrm{d}y} + C_1, \tag{3.18}$$

where $W_\infty(y) = W(1/y)$ [11]. By expressing the superpotential $W_\infty(y)$ in a power series of y,

$$W_\infty(y) = \sum_{j=0}^{\infty} \alpha_j y^j, \tag{3.19}$$

substituting this series into (3.18), and comparing equal powers of y, the series about $y = 0$ (i.e. $x \to \infty$) can be obtained, with the coefficients α_j given by

$$\alpha_0 = \sqrt{\frac{C_1}{1-q}}, \tag{3.20}$$

$$\alpha_1 = 0, \tag{3.21}$$

$$\alpha_j = -(j-1)\left(\frac{1+\sqrt{q^{j-2}}}{1-\sqrt{q^{j-2}}}\right)\frac{\alpha_{j-1}}{2\alpha_0} - \frac{1}{2\alpha_0}\sum_{k=2}^{j-2}\alpha_k\alpha_{j-k}, \qquad \text{for} \quad j \geqslant 3. \tag{3.22}$$

It is worthy to remark that the coefficient α_2 cannot be determined in this way because it depends on the small-x behavior of the superpotential [11]. However, we will show later in this paper that α_2 can be evaluated with the two-point Padé approximation, which can capture the essence of the superpotential at both large and small x.

On the other hand, similar to other SIPs, the exact energies of SSSIPs can be obtained analytically from (2.9), (3.3) and (3.10):

$$E_n = C_1 \frac{1-q^n}{1-q}, \qquad n = 0, 1, 2, \ldots. \tag{3.23}$$

It is interesting to note that for SSSIPs

$$\lim_{n\to\infty} E_n \equiv E_\infty = \frac{C_1}{1-q} = \lim_{x\to\infty} W^2(x). \tag{3.24}$$

The result is physically plausible and imposes a useful constraint on the asymptotic behavior of $W(x)$.

4. One-point Padé approximation

As discussed above, the series expansion of $W(x)$ in (3.15) diverges for $|x| > R_c$ and is not suitable for evaluation of W at large $|x|$. In addition, by virtue of (3.24), the superpotential $W(x)$ is expected to converge to a finite limit $E_\infty^{1/2}$ as $x \to \infty$. In order to remedy the divergence of the series in (3.15) and to ensure correct asymptotic behavior of $W(x)$ as well, we propose here to use the symmetric (or homogeneous) Padé approximation to construct the superpotential.

Generally speaking, the $[N/M]$ Padé approximant of a power series $\sum a_k x^k$ is a rational function of the form (see, e.g., [19])

$$\mathcal{P}_M^N(x) = \frac{\sum_{n=0}^{N} A_n x^n}{\sum_{m=0}^{M} B_m x^m}. \tag{4.1}$$

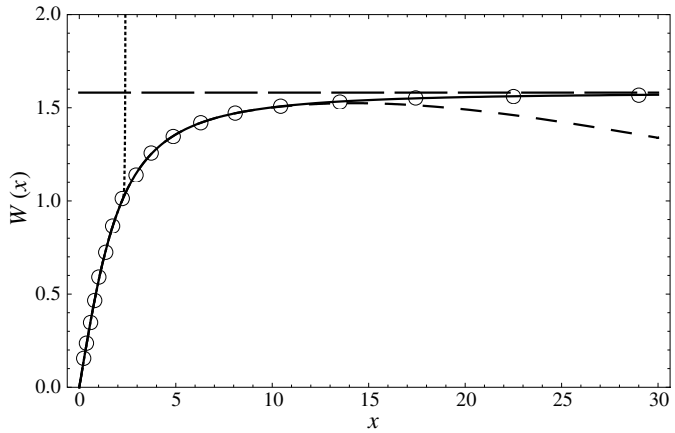

Figure 2. The superpotential $W(x)$ of SSSIP with $q = 0.6$ obtained from the exact numerical method (circles), power series expansion about $x = 0$ (dotted line, 60 leading terms were included in the sum), [20/20] one-point Padé approximant about $x = 0$ (short dashed line) and [10/10] two-point Padé approximant about $x = 0$ and $x = \infty$ (solid line) are plotted against x. Besides, the horizontal long dashed line shows the asymptotic value of $W(x)$ at $x = \infty$.

Here, A_n $(n = 0, 1, \ldots, N)$ and B_m $(m = 0, 1, \ldots, M)$ are constants to be determined from the coefficients of the power series by requiring that

$$\left(\sum_{k=0}^{\infty} a_k x^k\right)\left(\sum_{m=0}^{M} B_m x^m\right) \approx \sum_{n=0}^{N} A_n x^n. \tag{4.2}$$

The above equality holds approximately in the sense that the coefficients of the leading $(M + N + 1)$ terms on the lhs match the corresponding ones on the rhs. Without loss of generality, the choice $B_0 = 1$ is always assumed.

To generate an appropriate Padé approximant for $W(x)$, which approaches a constant value as $x \to \infty$, we consider a symmetric (or homogeneous) Padé approximant with $M = N$:

$$T_N(x) \equiv \mathcal{P}_N^N(x) = \frac{\sum_{k=0}^{N} A_k x^k}{\sum_{k=0}^{N} B_k x^k}. \tag{4.3}$$

Obviously, such a homogeneous Padé approximant tends to a constant A_N/B_N in the large-x limit. This point provides a strong motivation for us to construct $[N/N]$ Padé approximants for $W(x)$. In figures 2 and 3 (4 and 5), we show the superpotential $W(x)$ (the potential $V_1(x)$) constructed from the homogeneous Padé approximant about $x = 0$ (the short dashed line) for SSSIPs with $q = 0.6, 0.2$ and a comparison is made with the results obtained from the exact numerical integration method mentioned above (the circles). As shown in these figures, the Padé approximant shows good agreement with the exact numerical result for small x. More interestingly, unlike the Taylor series expansion of $W(x)$ about $x = 0$ (denoted by the dotted line in these figures), which diverges for x greater than R_c , the homogeneous Padé approximant is well behaved even if $|x| > R_c$ and gradually approaches the asymptotic value of $W(x)$, $E_\infty^{1/2}$ (the horizontal long dashed line), at intermediate values of x. However, the Padé approximant about $x = 0$ obviously fails to predict the correct asymptotic value of $W(x)$ for very large values of $|x|$ (see figures 2 and 3), which is a direct consequence of the fact that in general $A_N/B_N \neq E_\infty^{1/2}$.

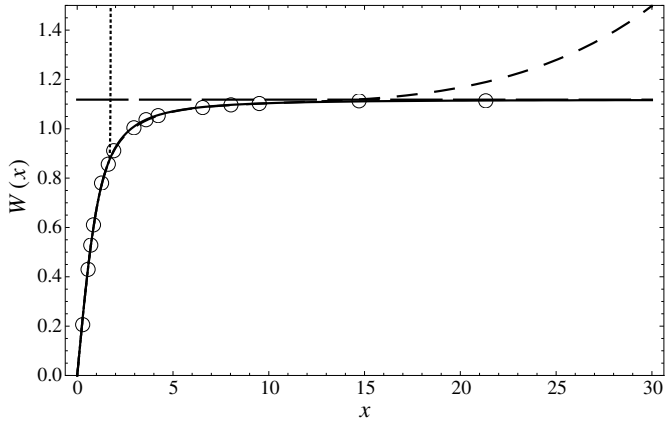

Figure 3. The superpotential $W(x)$ of SSSIP with $q = 0.2$ obtained from the exact numerical method (circles), power series expansion about $x = 0$ (dotted line, 60 leading terms were included in the sum), [22/22] one-point Padé approximant about $x = 0$ (short dashed line) and [10/10] two-point Padé approximant about $x = 0$ and $x = \infty$ (solid line) are plotted against x. Besides, the horizontal long dashed line shows the asymptotic value of $W(x)$ at $x = \infty$.

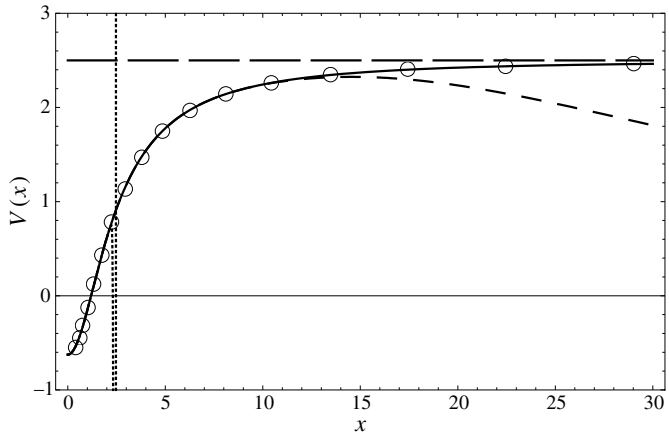

Figure 4. The potential $V_1(x)$ of SSSIP with $q = 0.6$ is plotted against x. The value of $V_1(x)$ is evaluated with the superpotential $W(x)$ obtained from the exact numerical method (circles), power series expansion about $x = 0$ (dotted line, 60 leading terms were included in the sum), [20/20] one-point Padé approximant about $x = 0$ (short dashed line) and [10/10] two-point Padé approximant about $x = 0$ and $x = \infty$ (solid line), respectively. Besides, the horizontal long dashed line shows the asymptotic value of $V_1(x)$ at $x = \infty$.

It is worthy to remark that the discrepancy between the Padé approximant and the exact result in the large-x regime cannot be eliminated by simply increasing the order (i.e. the value of N) of the approximant. In fact, the approximant might even demonstrate erratic behavior (e.g., emergence of unexpected poles on or near the real x-axis) when N is large (see figure 6). Physically speaking, the Padé approximant introduced above is generated from the Taylor series expansion of $W(x)$ about $x = 0$, which does not contain enough information about the large-x behavior of $W(x)$. This is the culprit giving rise to the discrepancy.

In order to capture more information about the large-x behavior of $W(x)$, we construct another homogenous Padé approximant with a center $x_0 \neq 0$. Similar to the method mentioned

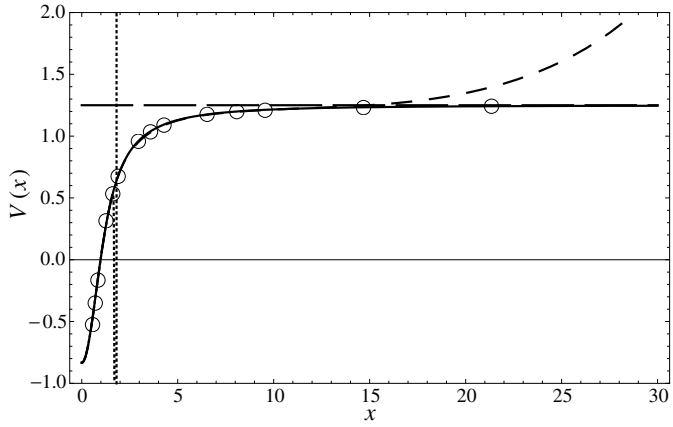

Figure 5. The potential $V_1(x)$ of SSSIP with $q = 0.2$ is plotted against x. The value of $V_1(x)$ is evaluated with the superpotential $W(x)$ obtained from the exact numerical method (circles), power series expansion about $x = 0$ (dotted line, 60 leading terms were included in the sum), [22/22] one-point Padé approximant about $x = 0$ (short dashed line) and [10/10] two-point Padé approximant about $x = 0$ and $x = \infty$ (solid line), respectively. Besides, the horizontal long dashed line shows the asymptotic value of $V_1(x)$ at $x = \infty$.

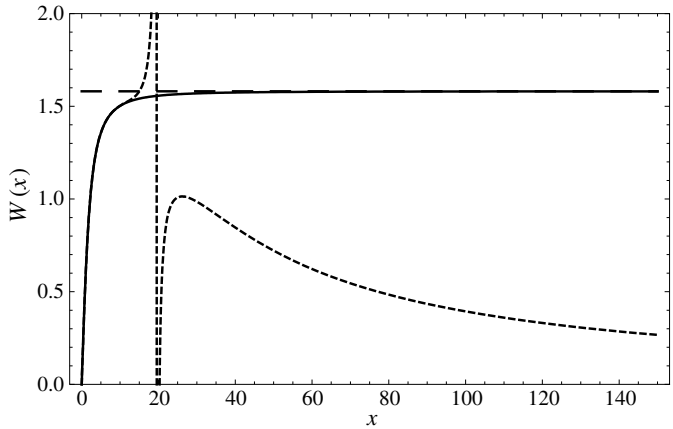

Figure 6. The superpotential $W(x)$ of SSSIP with $q = 0.6$ obtained from the [22/22] one-point Padé approximant about $x = 0$ (short dashed line) and [10/10] two-point Padé approximant about $x = 0$ and $x = \infty$ (solid line) are plotted against x, respectively. The horizontal long dashed line shows the asymptotic value of $W(x)$ at $x = \infty$. It is clearly shown that the one-point Padé approximant about $x = 0$ obviously fails to predict the correct asymptotic value of $W(x)$ for very large values of x. Besides, there are two singular points in the one-point Padé approximant around $x \simeq 20$ where the denominator vanishes.

above, a fraction of polynomials in $x - x_0$ is used to approximate the Taylor series expansion of $W(x)$ developed about $x = x_0$, namely,

$$T_N(x) = \frac{\sum_{k=0}^{N} A_k (x - x_0)^k}{\sum_{k=0}^{N} B_k (x - x_0)^k}$$
$$\approx W(x_0) + \frac{\mathrm{d}W(x = x_0)}{\mathrm{d}x}(x - x_0) + \frac{1}{2!}\frac{\mathrm{d}^2 W(x = x_0)}{\mathrm{d}x^2}(x - x_0)^2 + \cdots. \tag{4.4}$$

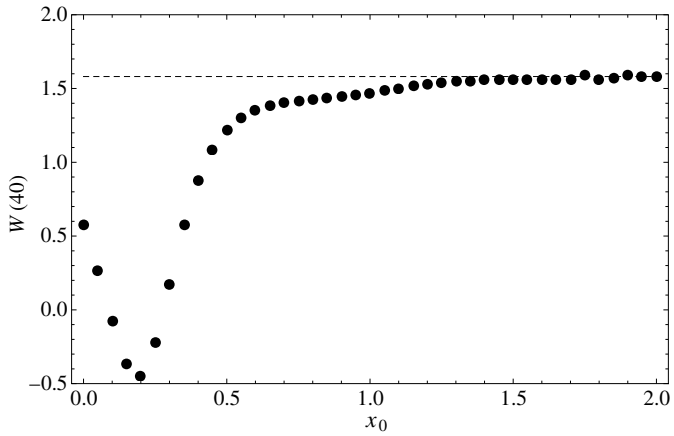

Figure 7. The value of $W(x = 40)$ for a SSSIP with $q = 0.6$ obtained from the [10/10] one-point Padé approximant centered at x_0 is plotted against x_0.

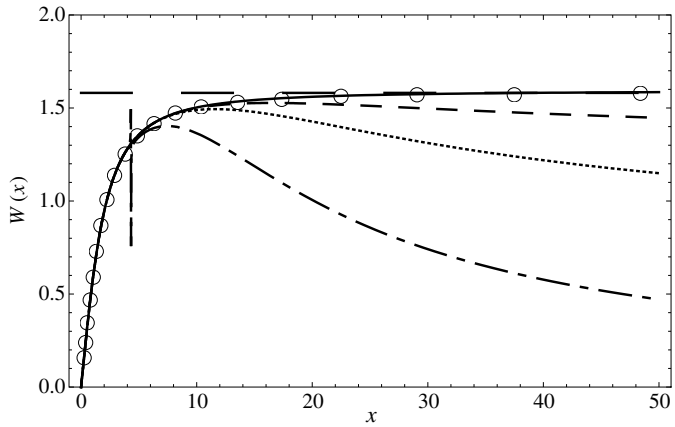

Figure 8. $W(x)$ for a SSSIP with $q = 0.6$ obtained from the [10/10] one-point Padé approximant centered at $x_0 = 0.0$ (dot-dashed line), 0.5 (dotted line), 1.0 (short dashed line) and 2.0 (solid line) are plotted against x. The horizontal long dashed line shows the asymptotic value of $W(x)$ in the large-x limit. For comparison, exact values of $W(x)$ (the circles) are also shown here.

The Taylor series of $W(x)$ in the above equation can be derived from (3.15), and again the coefficients A_k and B_k $(k = 0, 1, \ldots, N)$ can be determined from an equation analogous to (4.2). Since the superpotential is finite as $x \to \infty$, a homogeneous Padé approximant is adopted as in the previous case.

For the moment the choice of x_0 is completely free and there is no *a priori* argument to uniquely define it. On the other hand, as the superpotential $W(x)$ itself should be independent of the value of x_0, it is essential to choose an x_0 to respect this point. In figure 7 we show the values of the superpotential constructed from Padé approximants with different centers and evaluated at a point $x = 40$. The value of W varies greatly for approximants with x_0 close to zero; however, it becomes more stable if $x_0 \geqslant 1$. We then expect that the choice with $x_0 \geqslant 1$ is better than that with $x_0 \approx 0$. Such a least sensitivity criterion indeed provides a useful guideline for the choice of x_0. Figure 8 displays the numerical results of $W(x)$ constructed

from Padé approximants with different centers. It is obvious that the approximant with $x_0 = 2$ is much better than the approximant with $x_0 = 0$. The former choice yields accurate results even in the large-x regime, while the latter fails to do so in the same range.

5. Two-point Padé approximation

In order to construct a Padé approximant that can capture the essence of the superpotential in both the small and the large-x limits, represented respectively by the series in (3.15) and (3.19), we will use the two-point Padé approximation to achieve our purpose in the following discussion.

First of all, for the purpose of clarity, we let

$$W(x) = P_0 + P_1 x + P_2 x^2 + \cdots \equiv P(x), \tag{5.1}$$

$$W_\infty(y) = Q_0 + Q_1 y + Q_2 y^2 + \cdots \equiv Q(y), \tag{5.2}$$

where, as defined previously, $y = 1/x$. Second, we consider a $[N, N]$ homogeneous Padé approximant $T_N(x)$:

$$T_N(x) = \frac{A_0 + A_1 x + \cdots + A_N x^N}{B_0 + B_1 x + \cdots + B_N x^N}, \tag{5.3}$$

with the $2N + 1$ coefficients A_k and B_k to be determined as follows. When equating $T_N(x)$ to $P(x)$ around $x = 0$, we get the approximate equation

$$(A_0 + A_1 x + \cdots + A_N x^N) \approx (B_0 + B_1 x + \cdots + B_N x^N) P(x). \tag{5.4}$$

By comparing the coefficients of the leading $N + 1$ terms in each side, we deduce a matrix equation relating the coefficients A_k and B_k:

$$\begin{pmatrix} A_0 \\ A_1 \\ \vdots \\ A_N \end{pmatrix} = \begin{pmatrix} P_0 & 0 & 0 & 0 \\ P_1 & P_0 & 0 & 0 \\ \vdots & & \ddots & 0 \\ P_N & \cdots & \cdots & P_0 \end{pmatrix} \begin{pmatrix} B_0 \\ B_1 \\ \vdots \\ B_N \end{pmatrix}, \tag{5.5}$$

which can be accordingly written as $\vec{A} = \mathbf{P} \cdot \vec{B}$ in obvious matrix notations.

On the other hand, substituting $y = 1/x$ into (5.3) leads to a new fraction in the variable y:

$$\tilde{T}_N(y) \equiv T_N(1/x) = \frac{A_0 y^N + A_1 y^{N-1} + \cdots + A_N}{B_0 y^N + B_1 y^{N-1} + \cdots + B_N}. \tag{5.6}$$

$\tilde{T}_N(y)$ is expected to be close to $Q(y)$. Therefore, we have

$$(A_0 y^N + A_1 y^{N-1} + \cdots + A_N) \approx (B_0 y^N + B_1 y^{N-1} + \cdots + B_N) Q(y). \tag{5.7}$$

Again by comparing the coefficients of the leading $N + 1$ terms in each side of the above approximate equality, we find a matrix equation in the coefficients A_k and B_k:

$$\begin{pmatrix} A_0 \\ A_1 \\ \vdots \\ A_N \end{pmatrix} = \begin{pmatrix} Q_0 & Q_1 & \cdots & Q_N \\ 0 & \ddots & & \vdots \\ 0 & 0 & Q_0 & Q_1 \\ 0 & 0 & 0 & Q_0 \end{pmatrix} \begin{pmatrix} B_0 \\ B_1 \\ \vdots \\ B_N \end{pmatrix}, \tag{5.8}$$

which is compactly written as $\vec{A} = \mathbf{Q} \cdot \vec{B}$.

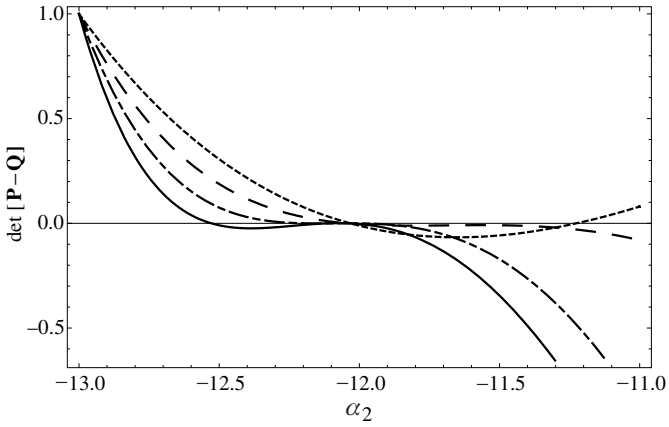

Figure 9. The determinant of the matrix $\mathbf{P} - \mathbf{Q}$ in the lhs of (5.10), which is normalized to unity at $\alpha_2 = -13$, is plotted against the parameter α_2 for a SSSIP with $q = 0.6$. [8/8] (dotted line), [10/10] (dashed line), [12/12] (solid line) and [14/14] (dot-dashed line) two-point Padé approximants are considered.

There are $2N + 2$ equations in (5.5) and (5.8). However, B_0 is equal to unity by convention. As a result, there are only $2N + 1$ undetermined coefficients, namely, $A_0, A_1, \ldots, A_N, B_1, B_2, \ldots, B_N$. At first sight, it seems that (5.5) and (5.8) together form an over-determined system. In fact, by comparing (5.5) with (5.8), we get

$$\begin{pmatrix} P_0 - Q_0 & -Q_1 & \cdots & -Q_N \\ P_1 & \ddots & & \vdots \\ \vdots & & P_0 - Q_0 & -Q_1 \\ P_N & \cdots & P_1 & P_0 - Q_0 \end{pmatrix} \begin{pmatrix} B_0 \\ B_1 \\ \vdots \\ B_N \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ \vdots \\ 0 \end{pmatrix} = \mathbf{0}, \tag{5.9}$$

or equivalently $(\mathbf{P} - \mathbf{Q}) \cdot \vec{B} = \mathbf{0}$. The condition for the existence of nonzero solution to (5.9) is obviously

$$\det(\mathbf{P} - \mathbf{Q}) = 0. \tag{5.10}$$

As mentioned in the derivation of the series expansion of $W_\infty(y)$, the coefficient α_2 (i.e. Q_2 in the matrix $\mathbf{Q}$) cannot be determined solely from the large-x behavior of $W(x)$. Therefore, equation (5.10) indeed provides a means to determine α_2, which is an extra bonus of the two-point Padé approximation introduced here. On the other hand, equation (5.10) is a nonlinear algebraic equation of α_2 and hence multiple solutions of α_2 (real or complex) can be found. To select an appropriate solution of α_2, we impose three criteria for determining α_2. (i) Since the superpotential is real-valued, α_2 must also be real. (ii) The coefficient α_2 depends on the asymptotic behavior of the superpotential and should be independent of the parameters artificially introduced in the Padé approximation. Therefore, the value of α_2 should be insensitive to the parameter N used in the approximation. However, most real roots of (5.10) are found to be sensitive to the value of N, which are not acceptable. Thus, one can make use of this criterion to narrow down the choices of α_2. (iii) To minimize the effect of α_2 on the result, the best value of α_2 should affect the determinant of $\mathbf{P} - \mathbf{Q}$ the least. As an example, in figure 9 we plot $\det(\mathbf{P} - \mathbf{Q})$ against the parameter α_2 for a SSSIP with $q = 0.6$. Taking the criteria mentioned above into consideration, one can easily see that the optimal value of α_2 is about -12.

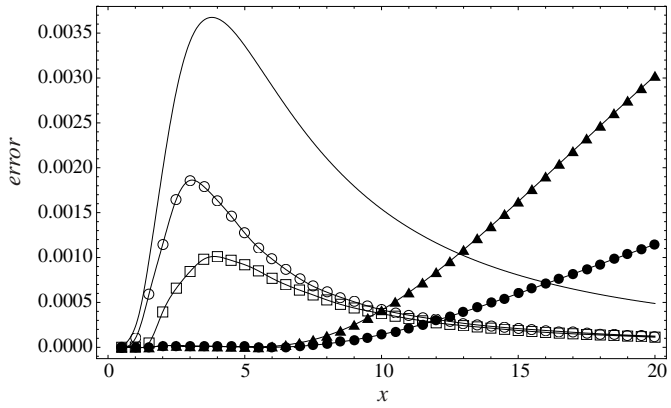

Figure 10. The errors in various Padé approximants of $W(x)$ are shown against x for the case with $q = 0.6$. The approximants considered here are, respectively, [10/10] (triangles) and [16/16] (solid dots) one-point Padé approximants about the center $x_0 = 2.0$, [6/6] (the solid line), [8/8] (empty circles) and [10/10] (empty squares) two-point Padé approximants. In this figure, the errors of [8/8] and [10/10] two-point Padé approximants are scaled up by ten times.

After fixing the coefficient α_2, the two-point Padé approximant in (5.3) can be constructed by rewriting the matrix equation in (5.9) as

$$B_0 \begin{pmatrix} P_1 \\ P_2 \\ \vdots \\ P_N \end{pmatrix} + \begin{pmatrix} P_0 - Q_0 & \cdots & -Q_{N-1} \\ \vdots & & \vdots \\ P_{N-1} & \cdots & P_0 - Q_0 \end{pmatrix} \begin{pmatrix} B_1 \\ B_2 \\ \vdots \\ B_N \end{pmatrix} = \mathbf{0}. \tag{5.11}$$

As $B_0 = 1$ by convention, other coefficients B_k $(1 \leqslant k \leqslant N)$ can be found:

$$\begin{pmatrix} B_1 \\ B_2 \\ \vdots \\ B_N \end{pmatrix} = - \begin{pmatrix} P_0 - Q_0 & \cdots & -Q_{N-1} \\ \vdots & & \vdots \\ P_{N-1} & \cdots & P_0 - Q_0 \end{pmatrix}^{-1} \begin{pmatrix} P_1 \\ P_2 \\ \vdots \\ P_N \end{pmatrix}. \tag{5.12}$$

Once $\vec{B}$ is obtained, $\vec{A}$ can be calculated from (5.5) or (5.8). Hence the two-point Padé approximant can be obtained.

In figures 2–5, we show the numerical results of two-point Padé approximants for the cases with $q = 0.6, 0.2$. It is clearly demonstrated in these figures that the two-point Padé approximant (the solid line) can yield accurate values of the superpotential and the potential for x in all ranges, in contrast to the one-point Padé approximant about $x = 0$ that deviates from the asymptotic value of $W(x)$ at large x. Besides, as shown in figure 6, the two-point Padé approximant is free of singularity. In figure 10, we compare the accuracies of the one-point and two-point Padé approximants of different orders. It is interesting to note that the error in two-point Padé approximants decreases with N rapidly and is particularly small for small or large values of x. (In figure 10, the errors of [8/8] and [10/10] two-point Padé approximants have been scaled up by ten times in order to make them more discernible in the figure.) Despite the fact that the one-point Padé approximant with an optimal choice of x_0 ($x_0 = 2$ in figure 10) can also yield accurate results for a large range of x, its error grows and is much greater than that of the two-point Padé approximant as x increases. Hence, we conclude

that the two-point Padé approximant provides an effective and accurate means to evaluate the superpotential.

6. Discussion and conclusion

We have demonstrated here the feasibility of the Padé approximation in evaluating the superpotential and the potential of SSSIPs. As is clearly shown in figures 2–5, the one-point Padé approximant generated from the series expansion of the superpotential at $x = 0$ can readily reproduce accurate numerical results for both the superpotential and the potential at small and intermediate x. In fact, its validity even goes beyond the radius of convergence of the original series. Furthermore, by judiciously choosing the center of expansion x_0, one can extend the validity of the one-point Padé approximant to a much larger range of x and eliminate its singular behavior as well (see figure 8).

Owing to the fact that the one-point Padé approximant can only sample the variation of the superpotential around the center of expansion x_0, the error of the one-point Padé approximant usually grows gradually in the large-x regime (see figure 10). Therefore, we propose to use the two-point Padé approximant, which can include the information about the superpotential in both small and large-x ranges, to remedy this drawback. As shown in figure 10, the two-point Padé approximant can indeed generate highly accurate numerical results in all ranges.

The method developed in the current paper can be adapted to consider other SSIPs with $R_n \neq 0$ for some $n \geqslant 2$. In fact, we have verified that the one-point Padé approximant works equally well for such SSIPs (not shown in the current paper). However, due to the fact that the asymptotic expansion for the superpotential of these SSIPs is, to our knowledge, unavailable, we cannot construct the two-point Padé approximant for them. Currently we are studying the possibility of expanding $W(x)$ about $x = \infty$ for these potentials and will report relevant progress in due course.

Lastly, as mentioned in section 1, the superpotential of SSSIPs can be used to construct the multi-soliton solution of the KdV equation (see, e.g., [13–18]). We expect our finding reported here can be applied in tandem with the theory of inverse scattering to generate time-dependent multi-soliton solutions of the KdV equation, which is also our next goal of endeavor.

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