Application of asymptotic iteration method to a deformed well problem

Hakan Ciftci[1,†] and H F Kisoglu[2,‡]

[1] Gazi Üniversitesi, Fen Fakültesi, Fizik Bölümü 06500 Teknikokullar Ankara, Türkiye
[2] Maritime Faculty, Department of Basic Sciences, Mersin University, Mersin, Turkey

(Received 23 June 2015; revised manuscript received 27 November 2015; published online 18 January 2016)

The asymptotic iteration method (AIM) is used to obtain the quasi-exact solutions of the Schrödinger equation with a deformed well potential. For arbitrary potential parameters, a numerical aspect of AIM is also applied to obtain highly accurate energy eigenvalues. Additionally, the perturbation expansion, based on the AIM approach, is utilized to obtain simple analytic expressions for the energy eigenvalues.

Keywords: asymptotic iteration method, quasi-exact solutions, perturbation method, approximate solutions

PACS: 02.30.Hq, 02.60.Cb, 03.65.Ge, 03.65.–w **DOI:** 10.1088/1674-1056/25/3/030201

1. Introduction

The solution of the Schrödinger equation, which is the main scope of quantum mechanics, depends upon the configuration of the system held, i.e., the behavior of the potential. One of the advantages of the asymptotic iteration method (AIM), introduced in Refs. [1] and [2], is that it can be applied to solve the eigenvalue problem exactly or approximately for numerous potentials.[3–14]

In the framework of perturbation theory, AIM has the advantage of obtaining simple analytic expressions for eigenvalues and eigenfunctions. Although, the standard perturbation theory allows us to construct both analytic expressions for the eigenvalues and the eigenfunctions, the eigenfunctions of the unperturbed Hamiltonian (the exactly solvable part) are essential for the construction. It is usually a challenging task to obtain expressions beyond the first order correction of the perturbative expansion. The advantage of AIM is that the coefficients in the perturbation expansions can be calculated directly without a prior knowledge of the exact eigenfunctions of the unperturbed Hamiltonian.[5,8,15–17]

In the present work, the AIM is used to obtain both the quasi-exact and approximate (numeric) solutions of the Schrödinger equation for a deformed well problem. A brief introduction to the AIM is summarized in Section 2. The approximate and quasi-exact eigenvalue solutions of the Schrödinger equation with the potential

$$V(x) = A\cos(x) + B^2\sin^2(x) + \frac{\gamma(\gamma+1)}{\sin^2(x)}, \quad x \in (0,\pi) \tag{1}$$

are obtained in Section 3, where A and B are real coefficients and γ ranges over the interval $(0,\infty)$. In Section 4, we apply the perturbation method in the framework of AIM to construct perturbative expansions for potential (1).

2. Asymptotic iteration method

In this section, we briefly outline the asymptotic iteration method, for more details we refer the reader to the original publication.[1] The AIM was introduced to solve the second-order homogeneous linear differential equations

$$y''(x) = \lambda_0(x)y'(x) + s_0(x)y(x), \tag{2}$$

where the functions λ_0 and s_0 have continuous derivatives in the domain of definition. According to the asymptotic aspect of the method, if

$$\frac{s_n}{s_{n-1}} = \frac{\lambda_n}{\lambda_{n-1}} \equiv \alpha \tag{3}$$

for sufficiently large $n > 0$, then the general solution of Eq. (2) reads

$$y(x) = \exp\left(-\int^x \alpha(t)\,\mathrm{d}t\right)\left[C_2 + C_1\int^x \exp\left(\int^t (\lambda_0(t)+2\alpha(t))\,\mathrm{d}\tau\right)\mathrm{d}t\right], \tag{4}$$

where

$$\lambda_n = \lambda'_{n-1} + s_{n-1} + \lambda_0\lambda_{n-1}, \qquad s_n = s'_{n-1} + s_0\lambda_{n-1}.$$

Eigenvalues E of the Schrödinger equation are the roots (zeros) of the following termination condition:

$$\delta_n(x) \equiv s_n(x)\lambda_{n-1}(x) - \lambda_n(x)s_{n-1}(x) = 0. \tag{5}$$

The eigenvalue problem (2) is said to be an exactly solvable (in a closed form) problem if the termination condition (5) is independent of the variable x. If $\delta_n \equiv \delta_n(E;x) = 0$, then a suitable initial value of x is necessary to start the AIM iteration. Such starting value may be found as the x coordinate of the minimum point of the potential $V(x)$.[3,5]

†Corresponding author. E-mail: hciftci@gazi.edu.tr
‡Corresponding author. E-mail: hasanfatihk@mersin.edu.tr

© 2016 Chinese Physical Society and IOP Publishing Ltd

3. The deformed well potential

In this section, we focus our attention on the deformed well potential

$$V(x) = A\cos(x) + B^2\sin^2(x) + \frac{\gamma(\gamma+1)}{\sin^2 x}, \quad x \in (0,\pi),$$

where A, B, and γ are the potential parameters and $\gamma \in [0,\infty)$. The one-dimensional Schrödinger equation then reads

$$\left\{\frac{\mathrm{d}^2}{\mathrm{d}x^2} + E - \left[A\cos(x) + B^2\sin^2(x) + \frac{\gamma(\gamma+1)}{\sin^2(x)}\right]\right\}\Psi(x) = 0,$$
$$\Psi(0) = \Psi(\pi) = 0. \tag{6}$$

Because of the vanishing of the wave function ψ at the end points, it is appropriate to assume the following form of Ψ:

$$\Psi(x) = \sin^{\gamma+1}(x)\, \mathrm{e}^{B\cos(x)} f(x). \tag{7}$$

Upon substituting Eq. (7) into Eq. (6), we directly obtain

$$f''(x) + 2\left[(\gamma+1)\frac{\cos(x)}{\sin(x)} - B\sin(x)\right] f'(x)$$
$$+ \left[E - (\gamma+1)^2 - \{A + B(2\gamma+3)\}\cos(x)\right] f(x) = 0. \tag{8}$$

This equation can be written using a change of the variable $x = \arccos y$ as

$$f''(y) = 2\left(\frac{\sigma y}{1-y^2} - B\right) f'(y) + \left(\frac{\xi y - \omega}{1-y^2}\right) f(y),$$
$$-1 < y < 1, \tag{9}$$

where $\omega = E - (\gamma+1)^2$, $\xi = A + 2\sigma B$, and $2\sigma = 2\gamma + 3$. The last equation is in a form suitable to initiate AIM sequences with

$$\lambda_0 = 2\left(\frac{\sigma y}{1-y^2} - B\right), \quad s_0 = \frac{\xi y - \omega}{1-y^2}. \tag{10}$$

3.1. Quasi-exact solutions

The first few iterations of $\delta_n(x) = s_n(x)\lambda_{n-1}(x) - \lambda_n(x)s_{n-1}(x)$ suggest the necessary condition $\xi = -2nB$ with $n = 0,1,2,\ldots$. Consequently, the two parameters A and B are related by the equation

$$A = -2B\left(n + \gamma + \frac{3}{2}\right), \quad n = 0,1,2,\ldots. \tag{11}$$

Thus for $n = 0$, we have

$$\xi = 0, \;\; w = 0 \quad \Rightarrow \quad E_0 = (\gamma+1)^2, \tag{12}$$

while for $n = 1$, we have

$$\xi = -2B, \;\; w = \sigma \mp \sqrt{\sigma^2 + 4B^2}, \tag{13}$$

which yields for the eigenvalues $E_1^{\pm}$ the following expressions:

$$E_1^- = \left(\gamma + \frac{3}{2}\right)^2 + \frac{1}{4} - \sqrt{\left(\gamma + \frac{3}{2}\right)^2 + 4B^2}, \tag{14}$$

$$E_1^+ = \left(\gamma + \frac{3}{2}\right)^2 + \frac{1}{4} + \sqrt{\left(\gamma + \frac{3}{2}\right)^2 + 4B^2}. \tag{15}$$

For higher values of n, the expressions for the eigenenergies become messy. However, the exact results can be immediately obtained for numerical values of the parameters (for example, $B = 1$ and $\sigma = 4.5$) as shown in the following table.

Table 1. Exact eigenvalues with $B = 1$ and $\sigma = 4.5$ for $n = 0,1,2,\ldots,5$ by using $\xi = -2nB$. Here k is sub-level for each n level and $k = 0,1,2,\ldots,n$.

n	k	ω_{nk}	E_{nk}
0	0	0	16.0000
1	0	–0.424429	15.5756
	1	9.42443	25.4244
2	0	–0.919071	15.0809
	1	9.27711	25.2771
	2	20.642	36.642
3	0	–1.47815	14.5218
	1	9.09552	25.0955
	2	20.6205	36.6205
	3	33.7621	49.7621
4	0	–2.09614	13.9039
	1	8.87768	24.8777
	2	20.5892	36.5892
	3	33.7953	49.7953
	4	48.834	64.834
5	0	–2.76786	13.2321
	1	8.62229	24.6223
	2	20.5459	36.5459
	3	33.8293	49.8293
	4	48.8905	64.8905
	5	65.8799	81.8799

3.2. Highly accurate eigenvalues for arbitrary parameters

For arbitrary potential parameters A, B, and γ, the termination condition (5) can be used to evaluate the eigenenergies with very high accuracy. In this case, however, the termination condition is a function of E and y. Thus an initial value of $y = y_0$ is necessary to start the AIM iteration. For the stability of AIM, it is sufficient to take $y_0 = 1/2$. In Table 2, we report the eigenenergies for $n = 0,1,2,\ldots,5$ and the parameters $(A;\ B;\ \gamma) = (0.167;0.0019;0.0019), (2;0.5;1), (4;1;1.97)$. As is seen from Table 2, the energy eigenvalues act as $\sim (n+\gamma+1)^2$.

Table 2. Approximately calculated eigenvalues $E_{\rm direct}$ for (A; B; γ) of (0.167; 0.0019; 0.0019), (2; 0.5; 1), and (4; 1; 1.97). The subscript represents the iteration number.

	$A=0.167, B=\gamma=0.0019$		$A=2, B=0.5, \gamma=1$		$A=4, B=1, \gamma=1.97$	
n	ω	$E_{\rm direct}$	ω	$E_{\rm direct}$	ω	$E_{\rm direct}$
0	-0.00231	$1.00149_{(3)}$	0.07399	$4.07399_{(10)}$	0.57328	$9.39418_{(13)}$
1	3.00473	$4.00853_{(4)}$	5.17104	$9.17104_{(12)}$	7.618	$16.4389_{(13)}$
2	8.008	$9.0118_{(5)}$	12.1609	$16.1609_{(11)}$	16.5264	$25.3473_{(14)}$
3	15.0116	$16.0154_{(6)}$	21.1506	$25.1506_{(13)}$	27.4331	$36.254_{(16)}$
4	24.0153	$25.0191_{(7)}$	32.1438	$36.1438_{(14)}$	40.348	$49.1689_{(18)}$
5	35.0191	$36.0229_{(8)}$	45.1392	$49.1392_{(15)}$	55.2698	$64.0907_{(19)}$

4. Perturbation theory within the frame of AIM

The theory of the perturbation method within AIM was introduced earlier in Ref. [17]; we give here a brief summary. Assume that the potential of a quantum system is written in the form

$$V(x)=V_0(x)+\mu V_{\rm p}(x), \tag{16}$$

where $V_0(x)$ is a solvable (or unperturbed Hamiltonian) potential, and $V_{\rm p}(x)$ and μ are the perturbed part and the perturbation expansion parameter, respectively. The Schrödinger equation then reads

$$\left(-\frac{{\rm d}^2}{{\rm d}x^2}+V_0(x)+\mu V_{\rm p}(x)\right)\Psi(x)=E\Psi(x). \tag{17}$$

The eigenvalues E_n can be written as the expansion of j-th order correction $E_n^{(j)}$

$$E_n=E_n^{(0)}+\mu E_n^{(1)}+\mu^2E_n^{(2)}+\cdots=\sum_{j=0}^{\infty}\mu^jE_n^{(j)}. \tag{18}$$

Using the substitution $\psi(x)=\psi_0(x)f(x)$ in Eq. (17), we obtain the following equation for $f(x)$:

$$f''(x)=\lambda_0(x,\mu,E)f'(x)+s_0(x,\mu,E)f(x). \tag{19}$$

The termination condition, Eq. (5), is written as

$$\begin{aligned}\delta_n(x,\mu,E) &= s_n(x,\mu,E)\lambda_{n-1}(x,\mu,E)\\ &\quad-\lambda_n(x,\mu,E)s_{n-1}(x,\mu,E)=0.\end{aligned}$$

Taylor's expansion of $\delta_n(x,\mu,E)$ about $\mu=0$ yields

$$\begin{aligned}\delta_n(x,\mu,E) &= \delta_n(x,0,E)+\frac{\mu}{1!}\frac{\partial\delta_n(x,\mu,E)}{\partial\mu}\bigg|_{\mu=0}\\ &\quad+\frac{\mu^2}{2!}\frac{\partial^2\delta_n(x,\mu,E)}{\partial\mu^2}\bigg|_{\mu=0}+\cdots\\ &=\sum_{k=0}^{\infty}\mu^k\delta_n^{(k)}(x,E),\end{aligned} \tag{20}$$

where

$$\delta_n^{(k)}(x,E)=\frac{1}{k!}\frac{\partial^k\delta_n(x,\mu,E)}{\partial\mu^k}\bigg|_{\mu=0}.$$

The necessary condition

$$\delta_n^{(k)}(x,E)=0 \tag{21}$$

can be obtained by means of Eq. (20) for each k. According to the perturbation method within the framework of AIM, solving the equation $\delta_n(x,0,E)=0$ with respect to (unknown) E gives $E_n^{(0)}$ (eigenvalues of the unperturbed Hamiltonian), equation $\delta_n^{(1)}(x,E)=0$ gives $E_n^{(1)}$ (the first-order correction to E_n), $\delta_n^{(2)}(x,E)$ gives $E_n^{(2)}$ (the second-order correction to E_n), and so on. The eigenfunctions can be easily found in a similar manner. This is an attractive feature of the AIM that allows us to obtain the eigenfunctions $f_n(x)$ without any prior knowledge of the exact solutions of the unperturbed Hamiltonian, given as follows:

$$f_n(x)=\exp\left(-\int^x\alpha_n(t,\mu)\,{\rm d}t\right), \tag{22}$$

where $\alpha_n(t,\mu)\equiv s_n(t,\mu)/\lambda_n(t,\mu)$. Let

$$\alpha_n(t,\mu)=\sum_{k=0}^{\infty}\mu^k\alpha_n^{(k)}(t), \tag{23}$$

where

$$\alpha_{n(x)}^{(k)}=\frac{1}{k!}\frac{\partial^k\alpha_{n(x,\mu)}}{\partial\mu^k}\bigg|_{\mu=0}.$$

Thus, the perturbation expansion of $f_{n(x)}$ can be written as

$$f_n(x)=\exp\left[\sum_{k=0}^{\infty}\mu^k\left(-\int^x\alpha_n^{(k)}(t)\,{\rm d}t\right)\right]=\prod_{k=0}^{\infty}f_n^{(k)}(x), \tag{24}$$

where the k-th order correction $f_n^{(k)}(x)$ to $f_n(x)$ is

$$f_n^{(k)}(x)=\exp\left[\mu^k\left(-\int^x\alpha_n^{(k)}(t)\,{\rm d}t\right)\right],\quad k=0,1,2,\ldots. \tag{25}$$

4.1. Perturbative expansion

In Section 3, we have obtained the eigenvalue equation in the appropriate form for AIM application as

$$f''(y)=2\left(\frac{\sigma y}{1-y^2}-B\right)f'(y)+\left(\frac{\xi y-\omega}{1-y^2}\right)f(y),$$

where $\omega=E-(\gamma+1)^2$, $\xi=A+2\sigma B$, and $2\sigma=2\gamma+3$. Parameters A and B of the potential $V(x)$, given by Eq. (1), are related to each other via the relation (11). Suppose that $A=2aB$,

in this case, $\xi = 2(a+\sigma)B$ for some values of a, then we have the following differential equation for $f(y)$:

$$f''(y) = 2\left(\frac{\sigma y}{1-y^2} - B\right) f'(y) + \left(\frac{2(a+\sigma)By - \omega}{1-y^2}\right) f(y), \tag{26}$$

where B can be regarded as a perturbation expansion parameter. By expanding ω as follows:

$$\omega_n = \omega_n^{(0)} + B\omega_n^{(1)} + B^2\omega_n^{(2)} + \cdots, \tag{27}$$

the general form of the zeroth order correction $\omega_n^{(0)}$ is obtained

$$\delta^{(0)}(x, 0, \omega_n^{(0)}) = 0, \tag{28}$$

as mentioned previously. It is not difficult to solve this equation for $\omega_n^{(0)}$, where the first few iterations yield 0, 2σ, $2+4\sigma$, $6+6\sigma$, $12+8\sigma$, $20+10\sigma$, and in general, one can write

$$\omega_n^{(0)} = n(n-1) + 2n\sigma, \qquad n = 1, 2, \ldots. \tag{29}$$

The first-order correction to ω_n is generalized in a similar manner, and it is found that $\omega_n^{(1)} = 0$ for each n level via the equation $\delta^{(1)}(x, 0, \omega_n^{(1)}) = 0$. The second-order correction to ω_n is generalized as

$$\omega_n^{(2)} = -2\left(\frac{a^2 g_1(n,\sigma) - g_2(n,\sigma)}{g_3(n,\sigma)}\right), \tag{30}$$

where

$$\begin{aligned} g_1(n,\sigma) &= 2\sigma^2 - (2n+5)\sigma - \left(n^2 - n - 3\right), \\ g_2(n,\sigma) &= 2\sigma^4 + (6n-5)\sigma^3 + \left(7n^2 - 11n + 3\right)\sigma^2 \\ &\quad + 4n(n-1)^2\sigma + n^2(n-1)^2, \\ g_3(n,\sigma) &= (2\sigma + 2n + 1)(2\sigma + 2n - 3)(\sigma + n)(\sigma + n - 1). \end{aligned}$$

If equations (29) and (30) are substituted in Eq. (27), one can obtain

$$\omega_n = n(n-1) + 2n\sigma - \left(\frac{A^2 g_1(n,\sigma) - 4B^2 g_2(n,\sigma)}{2g_3(n,\sigma)}\right), \tag{31}$$

where we use $a = A/2B$. Using $\omega_n = E_n - (\gamma+1)^2$, we obtain approximate E_n^{p} (perturbed energy) as follows:

$$E_n^{\mathrm{p}} \approx (\gamma + n + 1)^2 - \left(\frac{A^2 g_1(n,\sigma) - 4B^2 g_2(n,\sigma)}{2g_3(n,\sigma)}\right). \tag{32}$$

Some numeric results of this formula are given in Table 3 for $n = 0, 1, 2, \ldots, 5$, and in Table 4 for $n = 0, 1, 2, \ldots, 10$. The comparison of E_n^{p} with direct evaluation E_{direct} using AIM for arbitrary A, B, and γ is also given in Tables 3 and 4. The subscripts represent the iteration numbers in both tables.

Table 3. Comparison of eigenvalues of perturbed Hamiltonian E_n^{p} with numerical ones E_{direct} for $A = 2$, $B = 2$, $\gamma = 4$, and $n = 0, 1, 2, \ldots, 5$.

n	ω_n	E_{direct}	E_n^{p}
0	3.6259	$28.6259_{(13)}$	28.6364
1	14.1219	$39.1219_{(14)}$	39.1329
2	26.8245	$51.8245_{(17)}$	51.8308
3	41.6323	$66.6323_{(18)}$	66.6353
4	58.5005	$83.5005_{(19)}$	83.5015
5	77.406	$102.406_{(19)}$	102.406

Table 4. Comparison of the eigenvalues of perturbed Hamiltonian E_n^{p} with numerical ones E_{direct} for $A = 2$, $B = 1$, $\gamma = 0.0019$, and $n = 0, 1, 2, \ldots, 10$.

n	ω_n	E_{direct}	E_n^{p}
0	0.38637	$1.39017_{(12)}$	1.42145
1	3.65921	$4.66301_{(13)}$	4.64073
2	8.56603	$9.56983_{(16)}$	9.56855
3	15.5445	$16.5483_{(15)}$	16.547
4	24.5364	$25.5402_{(16)}$	25.5392
5	35.5338	$36.5376_{(18)}$	36.5368
6	48.5336	$49.5374_{(18)}$	49.5369
7	63.5349	$64.5387_{(19)}$	64.5383
8	80.537	$81.5408_{(20)}$	81.5404
9	99.5392	$100.543_{(20)}$	100.543
10	120.542	$121.546_{(21)}$	121.546

It is easily seen from Table 3 that the AIM values E_{direct} are consistent with the perturbation results E_n^{p}. Also, they become more consistent as the energy level n increases, although the values of E_{direct} converge more slowly. Similar comments apply to the results reported in Table 4 as well. Furthermore, the eigenvalues act as $\sim (n+\gamma+1)^2$ while $\omega_n \approx n(n+2)$ in Table 4. In Table 5, values of E_{direct} and E_n^{p} are inconsonant for $A = B = 5$ and $\gamma = 0.5$.

Table 5. Comparison of the eigenvalues of perturbed Hamiltonian E_n^{p} with numerically calculated ones E_{direct} for $A = B = 5$, $\gamma = 0.5$, and $n = 0, 1, 2, \ldots, 5$. The subscripts represent the iteration numbers.

n	ω_n	E_{direct}	E_n^{p}
0	11.8935	$14.1435_{(31)}$	21.0000
1	19.3048	$21.5548_{(34)}$	20.8333
2	25.0743	$27.3243_{(36)}$	25.7917
3	32.0111	$34.2611_{(40)}$	33.375
4	41.5015	$43.7515_{(37)}$	43.1667
5	53.2222	$55.4722_{(39)}$	55.0476

5. Conclusion

We have used AIM to solve the Schrödinger equation with a deformed well potential represented by a trigonometric function. The application of AIM to this class of problem allows us to obtain the quasi-exact solutions under certain conditions on

the potential parameters. The method was also used to obtain accurate eigenvalues for arbitrary potential parameters. Generally speaking, the energy eigenvalues seem to behave as $\sim (n+\gamma+1)^2$ for larger quantum number n, see Eq. (32). Another usage of AIM is its perturbation version. In the standard perturbation theory, the eigenfunctions of the unperturbed Hamiltonian are essential to constructing the perturbation expansion for either energy eigenvalues or eigenfunctions. Also, determining the third and fourth order correction terms is a serious challenge. The advantage of the AIM perturbative approach is that the coefficients in the perturbation expansion can be calculated directly without the necessity of the analytic solutions of the unperturbed Hamiltonian. The numerical results show high consistency between the eigenvalues as obtained by the perturbation approach and those obtained by direct application of AIM. Although there is a slight shifting in the result obtained by the perturbation expansion for small values of n, such inconsistency tends to decrease as n increases.

References

[1] Ciftci H, Hall R L and Saad N 2003 *J. Phys. A: Math. Gen.* **36** 11807
[2] Ciftci H, Hall R L and Saad N 2005 *J. Phys. A: Math. Gen.* **38** 1147
[3] Ciftci H, Hall R L and Saad N 2013 *Cent. Eur. J. Phys.* **11** 37
[4] Ozer O and Levai G 2012 *Rom. Journ. Phys.* **57** 582
[5] Champion B, Hall R L and Saad N 2008 *Int. J. Mod. Phys. A* **23** 1405
[6] Falaye B J, Hamzavi M and Ikhdair S M 2013 *Chin. Phys. Lett.* **30** 020305
[7] Aygun M, Bayrak O and Boztosun I 2007 *J. Phys. B: At. Mol. Opt. Phys.* **40** 537
[8] Ciftci H, Hall R L and Saad N 2005 *Phys. Rev. A* **72** 022101
[9] Turbiner A V 2012 *J. Phys. A: Math. Gen.* **45** 025203
[10] Ozer O 2009 *Progress of Theoretical Physics* **121** 437
[11] Yahiaoui S A and Bentaiba M 2011 *Acta Physica Polonica B* **42** 1755
[12] Hall R L, Saad N, Sen K D and Ciftci H 2009 *Phys. Rev. A* **80** 032507
[13] Ciftci H, Hall R L, Saad N and Dogu E 2010 *J. Phys. A: Math. Theor.* **43** 415206
[14] Bayrak O and Boztosun I 2006 *J. Phys. A: Math. Gen.* **39** 6955
[15] Ciftci H, Hall R L and Saad N 2005 *J. Phys. A: Math. Gen.* **39** 2338
[16] Barakat T 2006 *J. Phys. A: Math. Gen.* **39** 823
[17] Ciftci H, Hall R L and Saad N 2005 *Phys. Lett. A* **340** 388