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

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

are obtained in Section 3, where A and B are real coefficients and \( \gamma \) 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

\[ y''(x) = \lambda_0(x)y'(x) + s_0(x)y(x), \]  

where the functions \( \lambda_0 \) and \( s_0 \) have continuous derivatives in the domain of definition. According to the asymptotic aspect of the method, if

\[ \frac{s_n}{s_{n-1}} = \frac{\lambda_n}{\lambda_{n-1}} \equiv \alpha \]  

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

\[ y(x) = \exp \left( -\int^{x} \alpha(t) \, dt \right) \left[ C_2 + C_1 \int^{x} \exp \left( \int^{t} (\lambda_0(t) + 2 \alpha(t)) \, dt \right) \, dt \right], \]

where

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

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

\[ \delta_n(x) \equiv s_n(x)\lambda_{n-1}(x) - \lambda_n(x)s_{n-1}(x) = 0. \]

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]
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 \( \gamma \) are the potential parameters and \( \gamma \in [0, \infty) \). The one-dimensional Schrödinger equation then reads

\[ \frac{d^2 \Psi}{dx^2} + E - \left[ A \cos(x) + B^2 \sin^2(x) + \frac{\gamma (\gamma + 1)}{\sin^2(x)} \right] \Psi(x) = 0, \]

\[ \Psi(0) = \Psi'(\pi) = 0. \quad (6) \]

Because of the vanishing of the wave function \( \Psi \) at the end points, it is appropriate to assume the following form of \( \Psi \):

\[ \Psi(x) = \sin^{1+n}(x) e^{\theta \cos(x)} f(x). \quad (7) \]

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

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

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

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

\[ -1 < y < 1, \quad (9) \]

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

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

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

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

Thus for \( n = 0 \), we have

\[ \xi = 0, \quad w = 0 \quad \Rightarrow \quad E_0 = (\gamma + 1)^2, \quad (12) \]

while for \( n = 1 \), we have

\[ \xi = -2B, \quad w = \sigma + \sqrt{\sigma^2 + 4B^2}, \quad (13) \]

which yields for the eigenvalues \( E_1 \) the following expressions:

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

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

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.

| \( n \) | \( k \) | \( \omega_{nk} \) | \( E_{nk} \) |
|-------|-------|-----------------|--------|
| 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 |
| 6     | 0     | 65.8799         | 81.8799 |

3.2. Highly accurate eigenvalues for arbitrary parameters

For arbitrary potential parameters \( A, B, \) and \( \gamma \), 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 \( \gamma \). 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 \( A; \ B; \ \gamma = (0.167; 0.0019; 0.0019); (2; 0.5; 1); (4; 1.97) \). As is seen from Table 2, the energy eigenvalues act as \( \sim (n + \gamma + 1)^2 \).
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

\[ V(x) = V_0(x) + \mu V_p(x), \]

(16)

where \( V_0(x) \) is a solvable (or unperturbed Hamiltonian) potential, and \( V_p(x) \) and \( \mu \) are the perturbed part and the perturbation expansion parameter, respectively. The Schrödinger equation then reads

\[ \left( -\frac{d^2}{dx^2} + V_0(x) + \mu V_p(x) \right) \Psi(x) = E \Psi(x). \]

(17)

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

\[ E_n = E_n^{(0)} + \mu E_n^{(1)} + \mu^2 E_n^{(2)} + \cdots + \sum_{j=0}^{\infty} \mu^j E_n^{(j)}. \]

(18)

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

\[ f''(x) = \lambda_0(x, \mu, E) f(x) + s_0(x, \mu, E) f(x). \]

(19)

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

\[ \delta_n(x, \mu, E) = s_n(x, \mu, E) \lambda_{n-1}(x, \mu, E) - \lambda_n(x, \mu, E) s_{n-1}(x, \mu, E) = 0. \]

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

\[ \delta_n(x, \mu, E) = \delta_n(x, 0, E) + \frac{\mu}{1!} \frac{\partial \delta_n(x, \mu, E)}{\partial \mu} \bigg|_{\mu=0} + \frac{\mu^2}{2!} \frac{\partial^2 \delta_n(x, \mu, E)}{\partial \mu^2} \bigg|_{\mu=0} + \cdots \]

\[ = \sum_{k=0}^{\infty} \frac{\mu^k \delta_n^{(k)}(x, E)}{k!}. \]

(20)

The necessary condition

\[ \delta_n^{(k)}(x, E) = 0 \]

(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:

\[ f_n(x) = \exp \left( -\int x^\alpha_n(t, \mu) dt \right), \]

(22)

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

\[ \alpha_n(t, \mu) = \sum_{k=0}^{\infty} \mu^k \alpha_n^{(k)}(t), \]

(23)

where

\[ \alpha_n^{(k)}(t) = \frac{1}{k!} \frac{\partial^k \alpha_n(t, \mu)}{\partial \mu^k} \bigg|_{\mu=0}. \]

Thus, the perturbation expansion of \( f_n(x) \) can be written as

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

(24)

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

\[ f_n^{(k)}(x) = \exp \left[ \mu^k \left( -\int x^\alpha_n^{(k)}(t) dt \right) \right], \]

\[ k = 0, 1, 2, \ldots. \]

(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 $f(y)$:

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

(26)

where $B$ can be regarded as a perturbation expansion parameter. By expanding $\omega$ as follows:

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

(27)

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

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

(28)

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

$$
\omega_n^{(0)} = n(n - 1) + 2n\sigma, \quad n = 1, 2, \ldots \ldots
$$

(29)

The first-order correction to $\omega_n$ 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 $\omega_n$ is generalized as

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

(30)

where

$$
g_1(n, \sigma) = 2\sigma^2 - (2n + 5)\sigma - (n^2 - n - 3),
$$

$$
g_2(n, \sigma) = 2\sigma^4 + (6n - 5)\sigma^3 + (7n^2 - 11n + 3)\sigma^2 + 4n(n - 1)^2\sigma + n^2(n - 1)^2,
$$

$$
g_3(n, \sigma) = (2\sigma + 2n + 1)(2\sigma + 2n - 3)(\sigma + n)(\sigma + n - 1).
$$

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

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

(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:

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

(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 $E_{\text{direct}}$ using AIM for arbitrary $A$, $B$, and $\gamma$ is also given in Tables 3 and 4. The subscripts represent the iteration numbers in both tables.

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

| $n$ | $\omega_n$ | $E_{\text{direct}}$ | $E_n^p$ |
|-----|-------------|----------------------|--------|
| 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     | 36.5378 (18)         | 36.5368|
| 6   | 48.5336     | 49.5374 (18)         | 49.5369|
| 7   | 63.5349     | 64.5387 (19)         | 64.5383|
| 8   | 80.5377     | 81.5408 (20)         | 81.5404|
| 9   | 99.5392     | 100.543 (20)         | 100.543|
| 10  | 120.542     | 121.546 (21)         | 121.546|

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

It is easily seen from Table 3 that the AIM values $E_{\text{direct}}$ are consistent with the perturbation results $E_n^p$. Also, they become more consistent as the energy level $n$ increases, although the values of $E_{\text{direct}}$ 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 $E_{\text{direct}}$ and $E_n^p$ are inconsistent for $A = B = 5$ and $\gamma = 0.5$.

| $n$ | $\omega_n$ | $E_{\text{direct}}$ | $E_n^p$ |
|-----|-------------|----------------------|--------|
| 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|

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

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.

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