Calculation of the eigenfunctions and eigenvalues of Schrödinger type equations by asymptotic Taylor expansion method (ATEM)

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Abstract

A novel method is proposed to determine an analytical expression for eigenfunctions and numerical result for eigenvalues of the Schrödinger type equations, within the context of Taylor expansion of a function. Optimal truncation of the Taylor series gives a best possible analytical expression for eigenfunctions and numerical result for eigenvalues.

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I. INTRODUCTION

One of the source of progress of the sciences depends on the study of the same problem from different point of view. Besides their progress of the sciences those different point of views include a lot of mathematical tastes. Over the years considerable attention has been paid to the solution of Schrödinger equation. Determination of eigenvalues of the Schrödinger equation via asymptotic iteration method (AIM) has recently attracted some interest, arising from the development of fast computers [1–4]. This method have been widely applied to establish eigenvalues of the Schrödinger type equations [5–10]. Although the AIM formalism is very efficient to obtain eigenvalues of the Schrödinger equation, it requires tedious calculations in order to determine wave function if the system is not exactly solvable. When Schrödinger equation includes a non solvable potential, the calculation of wave function involved with a large number of terms will lose its simplicity and accuracy.

In this paper we will discuss new formalism based on the Taylor series expansion method, namely Asymptotic Taylor Expansion Method (ATEM). Although, Taylor Series Method [11] is an old one, it appears, however, not has been fully exploited in the analysis of both in solution of physical and mathematical problems. Yet, even today, new contributions to this problem are being made [12]. Apart from its formal relation to AIM, ATEM has also been easily applied to solve second order linear differential equations by introducing a simple computer program. We would like to mention here that the ATEM is a field of tremendous scope and has an almost unlimited opportunity, for its applications in the solution of the Schrödinger type equations. One can display a number of fruitful applications of the ATEM in different fields of the physics. For instance, our formalism of ATEM gives a new approach to the series solution of the differential equations as well as interrelation between series solution of differential equations and AIM. The method can also be applied to solve Dirac equation and Klein Gordon equation. In this paper we address ourselves to the solution of the eigenvalue problems by using the ATEM.

One of the fundamental advantage of ATEM is that (approximate) analytical expressions for the wave function of the associated Hamiltonian can easily be obtained. We note that ATEM also gives an accurate result for the eigenvalues when it is compared to AIM.

It should also be noted here that the determination of wave function by using AIM require tedious calculations if the system is not exactly solvable. For non exactly solvable potentials,
the calculation of wave function by using AIM involved with a large number of terms will lose
its simplicity and accuracy. Therefore, the method introduced here is useful to determine
an analytical expression for the wave function of the non exactly solvable equations.

The paper is organized as follows. The first main result of the paper is given in section by
reformulating the well known Taylor series expansion of a function. Section 3 is devoted to
the application of the main result for solving the Schrödinger equation including various poten-
tials. As a practical example, we illustrate solution of the Schrödinger equation including
anharmonic oscillator potential and the Hamiltonian of an interacting electron in a quantum
dot. In this section we present an approximate analytical expression for eigenfunction and
numerical results for eigenvalues of the anharmonic oscillator potential and the Hamiltonian
of an interacting electron in a quantum dot. We also analyze asymptotic behavior of the
Hamiltonian. Finally we comment on the validity of our method and remark on its possible
use in different fields of the physics in section 4.

II. A NEW FORMALISM OF THE TAYLOR EXPANSION METHOD

In this section, we show the solution of the Schrödinger equation for a quite ample class
of potentials, by modifying Taylor series expansion by means of a finite sequence instead
of an infinite sequence and its termination possessing the property of quantum mechanical
wave function. In quantum mechanics bound state energy of the atom is quantized and
eigenvalues are discrete and for each eigenvalues there exist one or more an eigenfunctions.
When we are dealing with the solution of the Schrödinger equation we are mainly interested
in the discrete eigenvalues of the problem. The first main result of this conclusion gives
necessary and sufficient conditions for the termination of the Taylor series expansion of the
wave function.

Let us consider Taylor series expansion of a function $f(x)$ about the point $a$:

$$f(x) = f(a) + (x - a)f'(a) + \frac{1}{2}(x - a)^2f''(a) + \frac{1}{6}(x - a)^3f^{(3)}(a) + \cdots$$

$$= \sum_{n=0}^{\infty} \frac{(x - a)^n}{n!}f^{(n)}(a)$$

where $f^{(n)}(a)$ is the $n^{th}$ derivative of the function at $a$. Taylor series specifies the value of
a function at one point, $x$, in terms of the value of the function and its derivatives at $a$.
reference point $a$. Expansion of the function $f(x)$ about the origin ($a = 0$), is known as Maclaurin’s series and it is given by,

$$f(x) = f(0) + xf'(0) + \frac{1}{2}x^2 f''(0) + \frac{1}{6}x^3 f^{(3)}(0) + \cdots = \sum_{n=0}^{\infty} \frac{x^n}{n!} f^{(n)}(0).$$

(2)

Here we develop a method to solve a second order linear differential equation of the form:

$$f''(x) = p_0(x)f'(x) + q_0(x)f(x).$$

(3)

It is obvious that the higher order derivatives of the $f(x)$ can be obtained in terms of the $f(x)$ and $f'(x)$ by differentiating (3). Then, higher order derivatives of $f(x)$ are given by

$$f^{(n+2)}(x) = p_n(x)f'(x) + q_n(x)f(x)$$

(4)

where

$$p_n(x) = p_0(x)p_{n-1}(x) + p'_{n-1}(x) + q_{n-1}(x), \quad \text{and}$$

$$q_n(x) = q_0(x)p_{n-1}(x) + q'_{n-1}(x).$$

(5)

Of course, the last result shows there exist a formal relation between AIM and ATEM. To this end, we conclude that the recurrence relations (5) allow us algebraic exact or approximate analytical solution of (3) under some certain conditions. Let us substitute (5) into the (1) to obtain the function that is related to the wave function of the corresponding Hamiltonian:

$$f(x) = f(0) \left(1 + \sum_{n=2}^{m} q_{n-2}(0) \frac{x^n}{n!}\right) + f'(0) \left(1 + \sum_{n=2}^{m} p_{n-2}(0) \frac{x^n}{n!}\right).$$

(6)

After all we have obtained an useful formalism of the Taylor expansion method. This form of the Taylor series can also be used to obtain series solution of the second order differential equations. In the solution of the eigenvalue problems, truncation of the the asymptotic expansion to a finite number of terms is useful. If the series optimally truncated at the smallest term then the asymptotic expansion of series is known as superasymptotic [13], and it leads to the determination of eigenvalues with minimum error.

Arrangement of the boundary conditions for different problems becomes very important because improper sets of boundary conditions may produce nonphysical results. When only odd or even power of $x$ collected as coefficients of $f(0)$ or $f'(0)$ and vice verse, the series
is truncated at \( n = m \) then an immediate practical consequence of these condition for 
\[ q_{m-2}(0) = 0 \text{ or } p_{m-2}(0) = 0. \]
In this way, the series truncates at \( n = m \) and one of the 
parameter in the \( q_{m-2}(0) \) or \( p_{m-2}(0) \) belongs to the spectrum of the Schrödinger equation.
Therefore eigenfunction of the equation becomes a polynomial of degree \( m \). Otherwise 
the spectrum of the system can be obtained as follows: In a quantum mechanical system 
eigenfunction of the system is discrete. Therefore in order to terminate the eigenfunction 
f(\( x \)) we can concisely write that

\[
q_m(0)f(0) + p_m(0)f'(0) = 0 \\
q_{m-1}(0)f(0) + p_{m-1}(0)f'(0) = 0
\]
(7)

eliminating \( f(0) \) and \( f'(0) \) we obtain

\[
q_m(0)p_{m-1}(0) - p_m(0)q_{m-1}(0) = 0
\]
(8)
again one of the parameter in the equation related to the eigenvalues of the problem.

We can state that the ATEM reproduces exact solutions to many exactly solvable differential equations and these equations can be related to the Schrödinger equation. It will be shown in the following section ATEM also gives accurate results for non-solvable Schrödinger equations, such as the sextic oscillator, cubic oscillator, deformed Coulomb potential, etc. which are important in applications to many problems in physics. This asymptotic approach opens the way to the treatment of Schrödinger type equation including large class of potentials of practical interest.

III. SOLUTION OF THE SCHRÖDINGER EQUATION BY USING ATEM

An analytical solution of the Schrödinger equation is of high importance in nonrelativistic quantum mechanics, because the wave function contains all necessary information for full description of a quantum system. In this section we take a new look at the solution of the Schrödinger equation by using the method of ATEM developed in the previous section. Let us consider the following eigenvalue problem \((\hbar = 2m = 1)\)

\[
-\frac{d^2\psi(x)}{dx^2} + V(x)\psi(x) = E\psi(x)
\]
(9)
where \( V(x) \) is the potential, \( \psi(x) \) is wave function and \( E \) is the energy of the system. The equation has been solved exactly for a large number of potentials by employing various tech-
niques. In general, it is difficult to determine the asymptotic behavior of (9) in the present form. Therefore it is worthwhile to transform (9) to an appropriate form by introducing the wave function \( \psi(x) = f(x) \exp\left(-\int W(x)dx\right) \). Thus, this change of wave function guarantees \( \lim_{x \to \infty} \psi(x) = 0 \). We recast (9) and we obtain the following equation

\[
L(x) = -f''(x) + 2W(x)f'(x) + (V(x) + W'(x) - W^2(x) - E)f(x) = 0. \tag{10}
\]

In this formalism of the equation coefficients in (3) can be expressed as:

\[
p_0(x) = 2W(x), \quad q_0(x) = (V(x) + W'(x) - W^2(x) - E).
\]

Using the relation given in (5) one can easily compute \( p_n(x) \) and \( q_n(x) \) by a simple MATHEMATICA program. Our task is now to illustrate the use of ATEM to obtain explicit analytical solution of the Schrödinger equation including various potentials.

1. **Anharmonic oscillator**

Solution of the Schrödinger equation including anharmonic potential has attracted a lot of attention, arising its considerable impact on the various branches of physics as well as biology and chemistry. The equation is described by the Hamiltonian

\[
H = -\frac{d^2}{dx^2} + x^2 + gx^4. \tag{11}
\]

In practice anharmonic oscillator problem is always used to test accuracy and efficiency of the unperturbative methods. Let us introduce, the asymptotic solutions of anharmonic oscillator Hamiltonian when \( W(x) = x \), then the wave function takes the form

\[
\psi = e^{-\frac{x^2}{2}} f(x),
\]

and (10) can be expressed as

\[
L(x) = -\frac{d^2f}{dx^2} + 2x \frac{df}{dx} + (gx^4 + 1 - E)f = 0. \tag{12}
\]

Comparing the equations (3) and (12) we can deduce that

\[
p_0(x) = 2x \text{ and } q_0(x) = (gx^4 + 1 - E). \tag{13}
\]
Here we take a new look at the solution of the (12) by using the method of ATEM developed in the previous section. By applying (8), the corresponding energy eigenvalues are calculated by the aid of a MATHEMATICA program.

The term asymptotic means the function approaching to a given value as the iteration number tends to infinity. By the aid of MATHEMATICA program we calculate eigenvalues $E$ and eigenfunction $f(x)$ for $g = 0.1$ using number of iterations $k = \{20, 30, 40, 50, 60, 70, 80\}$. The eigenvalues are presented in Table I and are compared with results computed by the AIM [1] and direct numerical integration method [14] by taking $g = 0.1$.

| $k$ | $n = 0$       | $n = 1$       | $n = 2$       | $n = 3$       | $n = 4$       | $n = 5$       |
|-----|---------------|---------------|---------------|---------------|---------------|---------------|
| 20  | 1.06529019    | 3.30632658    | 5.74394288    | 8.30136568    | 10.82233628   | 15.77123716   |
| 30  | 1.06528554    | 3.30688248    | 5.74807461    | 8.35361636    | 11.10902943   | 13.84616319   |
| 40  | 1.06528550    | 3.30687176    | 5.74795553    | 8.35266513    | 11.09828874   | 13.97716619   |
| 50  | 1.06528550    | 3.30687202    | 5.74795940    | 8.35267765    | 11.09860503   | 13.96951294   |
| 60  | 1.06528550    | 3.30687201    | 5.74795926    | 8.35267786    | 11.09859535   | 13.96995159   |
| 70  | 1.06528550    | 3.30687201    | 5.74795926    | 8.35267782    | 11.09859562   | 13.96992450   |
| 80  | 1.06528550    | 3.30687201    | 5.74795926    | 8.35267782    | 11.09859562   | 13.96992632   |
| $E$[1] | 1.065286     | 3.306871      | 5.747960      | 8.352642      | 11.09835      | 13.96695     |
| $E$[14]| 1.065286     | 3.306872      | 5.747959      | 8.352678      | 11.09860      | 13.96993     |

**TABLE I:** Eigenvalues of the (11) for different iteration numbers $k$ and $g = 0.1$. Last two rows corresponds the comparison of eigenvalues computed by the AIM [1], direct numerical integration method [14].

The function $f(x)$ for $n = 2$ state is given in (14).
As we mentioned before using ATEM we can obtain an analytical expression for the wave function of the Schrödinger equation. Substituting $E$ into (6) we get the wave function of the Schrödinger equation for the corresponding eigenvalues. Analytical expressions signal that ATEM produce an efficient result for the eigenfunction. For the first four states the plot of the normalized wave functions are given in Figure 1.

\begin{align*}
k = 30; f(x) &= 1 - 2.37404x^2 + 0.147996x^4 + 0.0193758x^6 \\
&\quad -1.73022 \times 10^{-3}x^8 - 5.18734 \times 10^{-5}x^{10} + 8.68491 \times 10^{-6}x^{12} \\
k = 50; f(x) &= 1 - 2.37398x^2 + 0.14797x^4 + 0.0193735x^6 \\
&\quad -1.73037 \times 10^{-3}x^8 - 5.19242 \times 10^{-5}x^{10} + 8.67726 \times 10^{-6}x^{12} \\
k = 80; f(x) &= 1 - 2.37398x^2 + 0.14797x^4 + 0.0193735x^6 \\
&\quad -1.73037 \times 10^{-3}x^8 - 5.19243 \times 10^{-5}x^{10} + 8.67725 \times 10^{-6}x^{12}
\end{align*}
2. Interacting electrons in a quantum dot

In this section we present a procedure to solve the Schrödinger equation of two interacting electrons in a quantum dot in the presence of an external magnetic field by using ATEM. The problem has been discussed in various articles \[15\text{-}17\]. Here we just solve the mathematical part of the problem. Without further discussion the Schrödinger equation for a quantum dot containing two electrons in the presence of the magnetic field \(B\) perpendicular to the dot is given by

\[
H = \sum_{i=1}^{2} \left( \frac{1}{2m_i} (P_i + eA(r_i))^2 + \frac{1}{2} m_i \omega_0^2 r_i^2 + \frac{e^2}{\varepsilon |r_2 - r_1|} \right)
\]  

(15)

Introducing relative and center of mass coordinates \(r = r_2 - r_1, \ R = \frac{1}{2}(r_1 + r_2)\) the Hamiltonian can be separated into two parts such that

\[
H = 2H_r + \frac{1}{2}H_R,
\]

where

\[
H_r = \frac{p^2}{2m^*} + \frac{1}{2} m^* \omega^2 r^2 + \frac{e^2}{2 \varepsilon r} + \frac{1}{2} \omega_c L_r,
\]

(16a)

\[
H_R = \frac{P^2}{2m^*} + \frac{1}{2} m^* \omega^2 R^2 + \frac{1}{2} \omega_c L_R.
\]

(16b)

Equation (16b) is the Hamiltonian of the harmonic oscillator, and it can be solved exactly. Let us turn our attention to the solution of the Hamiltonian \(H_r\). In the polar coordinate \(r = (r, \alpha)\), if the eigenfunction

\[
\phi = r^{-\frac{\ell}{2}} e^{i\ell \alpha} u(r)
\]

is introduced, the Schrödinger equation \(H \phi = E \phi\), can be expressed as

\[
\left( -\frac{\hbar^2}{2m^*} \frac{d^2}{dr^2} + \frac{\hbar^2}{2m^*} (\ell^2 - \frac{1}{4}) \frac{1}{r^2} + \frac{1}{2} m^* \omega^2 r^2 + \frac{e^2}{2 \varepsilon r} + \frac{1}{2} \omega_c L_r \right) u(r) = E u(r).
\]

(18)

From now on we restrict ourselves to the solution of Eq. (18). After changing the variable \(r \to \frac{\hbar}{\sqrt{2m^*}} r\) and substituting \(u(r) = r^{\ell+\frac{1}{2}} e^{-\frac{\hbar}{4 \varepsilon} r^2} f(r)\), we obtain the following equation

\[
L(r) = -rf''(r) + (\omega r^2 - (2\ell + 1)) f'(r) - (r E_n + \lambda) f(r) = 0,
\]

(19)

where

\[
E_r = E_n + (|\ell| + 1) \hbar \omega + \frac{1}{2} L_r \omega_c, \quad \lambda = -\frac{e^2}{2 \varepsilon},
\]

(20)

for simplicity we have chosen that \(\hbar \omega = \frac{\hbar^2}{2m^*} = 1\). In this case the functions \(p_0(r)\) and \(q_0(r)\) are given by

\[
p_0(r) = \omega r - \frac{2\ell + 1}{r} \quad \text{and} \quad q_0(r) = -E_n - \frac{\lambda}{r}.
\]

(21)
Meanwhile we bring to mind that Hamiltonian \( (15) \) possesses a hidden symmetry. This implies that the Hamiltonian is quasi-exactly solvable \([15, 16]\). Fortunately, quasi exact solvability of the Hamiltonian gives us an opportunity to check accuracy of our result and to test our method. In order to obtain quasi exact solution of \((19)\) we set in:

\[
E_n = j\omega, \text{ where } j = 1, 2, 3, \ldots
\]

and then the problem is exactly solvable when the following relation is satisfied:

\[
\lambda = \left\{ \pm \sqrt{\omega(2\ell + 1)} \right\}; j = 1 \\
\lambda = \left\{ 0, \pm \sqrt{2\omega(4\ell + 3)} \right\}; j = 2 \\
\lambda = \left\{ 0, \pm \sqrt{10\omega(\ell + 1) \pm \omega\sqrt{73 + 128\ell + 64\ell^2}} \right\}; j = 3 \\
\ldots
\]

Note that \(\lambda, \omega\) and \(\ell\) belong to the spectrum of the Hamiltonian. Therefore an accuracy check for the ATEM can be made. We have tested ATEM and the result are given by

\[
\lambda = \left\{ \pm \sqrt{\omega(2\ell + 1)} \right\}; j = 1; E_n = \omega; \\
f(r) = 1 \mp \sqrt{\frac{\omega}{2\ell + 1}} r \\
\lambda = \left\{ \pm \sqrt{2\omega(4\ell + 3)} \right\}; j = 2; E_n = 2\omega; \\
f(r) = 1 \mp \sqrt{\frac{2\omega(4\ell + 3)}{2\ell + 1}} r + \frac{\omega}{2\ell + 1} r^2.
\]

Consequently, we demonstrated that our approach is able to reproduce exact results for the exactly solvable second order differential equations. Let us turn our attention to the complete solution of the \((19)\). We have again used 80 iterations during the solution of the equation and controlled the stability of the eigenvalues. The results are given in Table II.

We go back \((6)\) to obtain the wave function of the equation of \((19)\) for various values of \(E\). Their plots are given in Figure 2.

**IV. CONCLUSION**

The basic features of our approach are to reformulate Taylor series expansion of a function for obtaining both eigenvalues and eigenfunctions of the Schrödinger type equations.
| $k$ | $n = 0$   | $n = 1$    | $n = 2$    | $n = 3$    | $n = 4$    | $n = 5$    |
|-----|-----------|-----------|-----------|-----------|-----------|-----------|
| 20  | 0.63844692| 0.81078941| 2.43413075| 2.80439505| 4.30282729| 4.81597264|
| 30  | 0.64590375| 0.80463157| 2.45078087| 2.79146457| 4.32486753| 4.79696796|
| 40  | 0.65007015| 0.80121630| 2.45998729| 2.78436605| 4.33697615| 4.78670663|
| 50  | 0.65279850| 0.79898546| 2.46598524| 2.77974956| 4.34484756| 4.78008225|
| 60  | 0.65475424| 0.79738773| 2.47027173| 2.77645083| 4.35046813| 4.77536829|
| 70  | 0.65624076| 0.79617357| 2.47352334| 2.77394739| 4.35473042| 4.77180017|
| 80  | 0.65741800| 0.79521187| 2.47609490| 2.77196620| 4.35810109| 4.76898147|

TABLE II: Eigenvalues $E_n$ of the (19) for different iteration numbers $k$ and $\lambda = \sqrt{\omega} = 1$ and $\ell = 1/2$.

FIG. 2: The wavefunctions of the two electron interacting in the harmonic oscillator potential field.

The parameters $\lambda = \sqrt{\omega} = 1$. 
Furthermore the technique given here has been applied to determine the eigenvalues and the eigenfunctions of the anharmonic oscillator and the Hamiltonian of two electrons in a quantum dot. We have shown that ATEM gives accurate results for eigenvalue problems.

As a further work ATEM can be developed in various directions. Position dependent mass Hamiltonians [18–20] can be solved by extending the method given in this paper. In particular, Lie algebraic or bosonic Hamiltonians can be solved within the framework of the method given here. Before ending this work a remark is in order. This extension leads to the solution of various matrix Hamiltonians, Dirac equation and Klein-Gordon equation. Our present results manifest that ATEM leads to the solution of the Schrödinger type equations in different fields of physics.

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