# Remarks on the Solution of the Position Dependent Mass (PDM) Schrödinger Equation

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## Abstract

An approximate method is proposed to solve position dependent mass Schrödinger equation. The procedure suggested here leads to the solution of the PDM Schrödinger equation without transforming the potential function to the mass space or vice verse. The method based on asymptotic Taylor expansion of the function, produces an approximate analytical expression for eigenfunction and numerical results for eigenvalues of the PDM Schrödinger equation. The results show that PDM and constant mass Schrödinger equations are not isospectral. The calculations are carried out with the aid of a computer system of symbolic or numerical calculation by constructing a simple algorithm.

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## INTRODUCTION

Quantum mechanical systems with a position dependent mass (PDM) generate interest for its relevance and importance in describing the physics of many microstructures of current interest, understanding transport phenomena in compositionally graded crystals, designing modern fabrication of nano devices such as quantum dots, wires and wells, developing theoretical models for effective interactions in nuclear physics, neutron stars, liquid crystals, metal clusters[1–15]. These applications have stimulated a naturally renewed interest in the solution of PDM quantum mechanical Hamiltonians. Recently, solution of the PDM Schrödinger equation, Dirac equation [16–19] and Klein-Gordon equation [20–22] have received much attention. A number of authors have studied PDM Schrödinger equation within the framework of point canonical transformations [23–26], Lie algebraic techniques[27–34], super symmetric quantum-mechanical [35–43], or other related techniques [44–63].

In most applications of such methods, PDM Schrödinger equation has been transformed in the form of the constant mass Schrödinger equation by changing coordinate and wave function. Obviously, this transformation generates isospectral potentials and exact solvability requirements result in constraints on the potential functions for the given mass distributions. In other words, a suitable transformation of coordinate and wave function becomes a bridge between constant mass and position dependent mass Schrödinger equation. As an example in a constant mass Schrödinger equation the choice of coordinate $u = \int_0^x \sqrt{m(x)}dx$ and wave function $\psi(u) = [2m(x)]^{1/4}\varphi(x)$ provides its transformation in the form of the PDM Schrödinger equation. In this case the potential is mass dependent; *i. e.* harmonic oscillator potential can be expressed as $V = \frac{1}{2}m\omega^2u^2 = \frac{1}{2}m\omega^2\left(\int_0^x \sqrt{m(x)}dx\right)^2$ and both constant and PDM Schrödinger equations have the same eigenvalues. The origin of such an isospectrality in the constant mass scenario has not yet been studied. It will be worthwhile to discuss physical acceptability of such an isospectrality in the position dependent mass background. In some articles [9–12, 21, 47, 53, 57, 61], solution of the PDM Schrödinger equation has been obtained without transforming the potential in to mass space . In this case the energy spectrum of the PDM Hamiltonians are not isospectral with the constant mass Hamiltonians. Therefore it is reasonable to develop a method for solving PDM Hamiltonian without transforming the potential into the mass space.

However, the fundamental question remains open: how the potential is affected when it

is expressed in the mass space? To answer this question, one has to obtain a solution for the Schrödinger equation without transforming the potential to the mass space. In this article, we will obtain a semi-analytical solution of the Schrödinger equation without transforming the potential to the mass space. This is another reason, to build a realistic model for solving PDM Hamiltonian.

It is well known that the study of the same mathematical problems from different point of view lead to the progress of the science and includes a lot of mathematical tastes. A technique based on asymptotic expansion of Taylor series [64] has recently been suggested to obtain eigenvalues of Schrödinger equation which improves both analytical and numerical determination of the eigenvalues. Asymptotic Taylor Expansion Method (ATEM) is very efficient to obtain eigenvalues of the Schrödinger equation because of their simplicity and low round off error. This method has been easily applied to establish eigenvalues and wave function of the Schrödinger type equations. 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 constant and PDM Schrödinger equations. In this paper, we address ourselves to the solution of the PDM Schrödinger equation by using the ATEM.

The paper is organized as follows. In the next section we review construction of ATEM by reformulating the well known Taylor series expansion of a function that satisfies second order homogeneous differential equation of the form: $f''(x) = p_0(x)f'(x) + q_0(x)f(x)$. Section 3 is devoted to the application of the main result for solving the PDM Schrödinger equation for various forms of the Kinetic energy operator. As a practical example, we illustrate solution of the PDM Schrödinger equation including harmonic oscillator potential and variable mass $m(x) = m_0\left(1 + \gamma x^2\right)$ [11]. In this section, we present an approximate analytical expression for eigenfunction and numerical results for eigenvalues of the PDM Schrödinger equation. We also analyze the asymptotic behavior of the Hamiltonian. Some concluding remarks are given in section 4.

## FORMALISM OF ATEM

In this section, we show the solution of the Schrödinger type 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. Let us consider Taylor series expansion [66] of a function $f(x)$ about the point $a$:

$$\begin{aligned} f(x) &= f(a) + (x-a)f'(a) + \frac{1}{2}(x-a)^2 f''(a) + \frac{1}{6}(x-a)^3 f^{(3)}(a) + ..... \\ &= \sum_{n=0}^{\infty} \frac{(x-a)^n}{n!} f^{(n)}(a) \end{aligned} \tag{1}$$

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,

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

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

$$f''(x) = p_0(x)f'(x) + q_0(x)f(x). \tag{3}$$

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

$$f^{(n+2)}(x) = p_n(x)f'(x) + q_n(x)f(x) \tag{4}$$

where

$$\begin{aligned} p_n(x) &= p_0(x)p_{n-1}(x) + p'_{n-1}(x) + q_{n-1}(x), \text{ and} \\ q_n(x) &= q_0(x)p_{n-1}(x) + q'_{n-1}(x). \end{aligned} \tag{5}$$

Of course, the last result shows there exist a formal relation between asymptotic iteration method (AIM) [70] and ATEM. We have observed that eigenfunction of the Schrödinger type equations can efficiently be determined by using ATEM. It is clear that the recurrence relations (5) allow us algebraic exact or approximate analytical expression for the solution of (3) under some certain conditions. Let us substitute (5) into the (1) to obtain

$$f(x) = f(0)\left(1 + \sum_{n=2}^{m} q_{n-2}(0)\frac{x^n}{n!}\right) + f'(0)\left(1 + \sum_{n=2}^{m} p_{n-2}(0)\frac{x^n}{n!}\right). \tag{6}$$

After all, we have obtained useful formalism of the Taylor expansion method. 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 [71], and it leads to the determination of eigenvalues with minimum error. Then boundary conditions can be applied as follows. 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 $q_{m-2}(0) = 0$ or $p_{m-2}(0) = 0$. In this way, one of the parameter in the $q_{m-2}(0)$ and/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

$$\begin{aligned} q_m(0)f(0) + p_m(0)f'(0) &= 0 \\ q_{m-1}(0)f(0) + p_{m-1}(0)f'(0) &= 0 \end{aligned} \tag{7}$$

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

$$q_m(0)p_{m-1}(0) - p_m(0)q_{m-1}(0) = 0 \tag{8}$$

again one of the parameter in the equation related to the eigenvalues of the problem.

In quantum mechanics bound state energy of the atom is quantized and eigenvalues are discrete and for each eigenvalues there exist one or more 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.

The process presented here is iterative and number of iteration is given by $m$. The results are obtained as follows: in our Mathematica program, we use an iteration number, say $m = 30$, then we obtain another result for $m = 40$, so on, then we compare values of the parameter (eigenvalue) in each case till 10 digits. If values of the parameter reach its asymptotic value then we use these values and omit the others. For instance, if one can obtain values of the parameters for $m = 40$, first few of them will be reached its asymptotic values, say first 8 values. The following comment for the function is considerable: for such a solution it is suitable to take sum of first 8 term in the (6).

It will be shown that ATEM gives accurate results for PDM Schrödinger equations. In the following sections, it is shown that this approach opens the way to the treatment of PDM Schrödinger equation including large class of potentials of practical interest.

## SOLUTION OF THE PDM SCHRÖDINGER EQUATION BY USING ATEM

In the PDM Schrödinger equation the mass and momentum operator no longer commute, so there are several ways to define kinetic energy operator. The general expression for the Hamiltonian with the kinetic energy operator introduced by von Roos[67] and potential energy $V(x)$, can be written as:

$$H = \frac{1}{4}\left(m^{\eta}\mathbf{p}m^{\varepsilon}\mathbf{p}m^{\rho} + m^{\rho}\mathbf{p}m^{\varepsilon}\mathbf{p}m^{\eta}\right) + V(x) \tag{9}$$

where $\eta + \varepsilon + \rho = -1$ is a constraint and $m = m(x)$ is position dependent mass. There are many debates for the choice of the parameters $\eta$, $\varepsilon$,and $\rho$, in our approach, we will obtain the solution of the PDM Schrödinger equation for the following Hamiltonians [67–69]:

$$H_1 = \frac{1}{2}\left(\mathbf{p}\frac{1}{m}\mathbf{p}\right) + V(x);\ \text{for } \varepsilon = -1, \rho = 0, \eta = 0, \tag{10a}$$

$$H_2 = \frac{1}{4}\left(\frac{1}{m}\mathbf{p}^2 + \mathbf{p}^2\frac{1}{m}\right) + V(x);\ \text{for } \varepsilon = 0, \rho = 0, \eta = -1, \tag{10b}$$

$$H_3 = \frac{1}{2}\left(\frac{1}{\sqrt{m}}\mathbf{p}^2\frac{1}{\sqrt{m}}\right) + V(x);\ \text{for } \varepsilon = -\frac{1}{2}, \rho = 0, \eta = -\frac{1}{2}, \tag{10c}$$

$$H_4 = \frac{1}{2}\left(\mathbf{p}\frac{1}{\sqrt{m}}\mathbf{p}\frac{1}{\sqrt{m}} + \frac{1}{\sqrt{m}}\mathbf{p}\frac{1}{\sqrt{m}}\mathbf{p}\right) + V(x);\ \text{for } \varepsilon = 0, \rho = -\frac{1}{2}, \eta = -\frac{1}{2}. \tag{10d}$$

Here we take a new look at the solution of the the PDM Schrödinger equation by using the method of ATEM developed in the previous section.

Before going further we share one of our significant observation during our calculations. If the mass distribution is not appropriate for a given potential, the eigenvalues do not reach their asymptotic values and resultant eigenfunction cannot be terminated when $x \to \pm\infty$. In order to illustrate semi analytical solution of the eigenvalue equations

$$H_i\psi(x) = E\psi(x), (i = 1, 2, 3, 4) \tag{11}$$

including harmonic oscillator potential, $V(x) = \frac{1}{2}m_0\omega^2x^2$, we use the mass distributions $m(x) = m_0\left(1 + \gamma x^2\right)$, where $\gamma$ is arbitrary positive constant. By the way, we emphasize

that the wave function of harmonic oscillator potential is well defined in the region of $\pm\infty$ and satisfy that $\lim_{x\to\pm\infty} \frac{|\psi(x)|^2}{\sqrt{m}} \to 0$. In this limit the mass distributions to be continuous.

It is well known that asymptotic behavior of constant mass Schrödinger equation including harmonic oscillator potential is given by $\psi = e^{-\frac{x^2}{2}} f(x)$, for simplicity we set $\hbar = m_0 = \omega = 1$.Thus, this change of wave function guaranties $\lim_{x\to\pm\infty} \frac{|\psi(x)|^2}{\sqrt{m}} \to 0$. After this transformation, we present an iteration algorithm to calculate both eigenvalues and eigenfunctions of the eigenvalue equation (11). Using this algorithm, we develop a Mathematica program, which demonstrates that it is easier to be implemented into a computer program, and produces a highly accurate solution with analytical expression efficiently.

*Asymptotic Analysis*

The term asymptotic means the function approaching to a given value as the iteration number tends to infinity. By the aid of a Mathematica program we calculate eigenvalues and eigenfunction of $H_1$ for $\gamma = 0.1$ using number of iterations $k = \{20, 30, 40, 50,60\}$. The function $f(x)$ for $n = 2$ state is given in (12) and eigenvalues are presented in Table I.

$$\begin{aligned}
k = 20;\ f(x) = \quad & 1 - 1.857x^2 - 1.619 \times 10^{-1}x^4 + 2.060 \times 10^{-2}x^6 \\
& +1.515 \times 10^{-3}x^8 - 1.261 \times 10^{-4}x^{10} - 6.495 \times 10^{-6}x^{12} \\
k = 40;\ f(x) = \quad & 1 - 1.856x^2 - 1.622 \times 10^{-1}x^4 + 2.051 \times 10^{-2}x^6 \\
& +1.505 \times 10^{-3}x^8 - 1.271 \times 10^{-4}x^{10} - 6.662 \times 10^{-6}x^{12} \qquad (12) \\
k = 60;\ f(x) = \quad & 1 - 1.856x^2 - 1.622 \times 10^{-1}x^4 + 2.051 \times 10^{-2}x^6 \\
& +1.504 \times 10^{-3}x^8 - 1.271 \times 10^{-4}x^{10} - 6.663 \times 10^{-6}x^{12}
\end{aligned}$$

Our calculation gives an accurate result for first 8 eigenvalues and eigenfunctions after 40 iterations. Here we have used 60 iterations. Figure 1 shows the plot of normalized wave functions for first 6 state.

*Solution of the Hamiltonians $H_2$, $H_3$ and $H_4$*

In the previous section we have illustrated applicability of our method by solving Hamiltonian $H_1$. In this section we apply the same procedure to solve the Hamiltonians $H_2$, $H_3$

| $k$ | $n=0$ | $n=1$ | $n=2$ | $n=3$ | $n=4$ | $n=5$ |
|---|---|---|---|---|---|---|
| 20 | 0.46889047 | 1.43341211 | 2.35765542 | 3.28397486 | 4.21360362 | 4.35399596 |
| 30 | 0.46889665 | 1.43348058 | 2.35642259 | 3.24660834 | 4.12086916 | 4.98321327 |
| 40 | 0.46889650 | 1.43348582 | 2.35655507 | 3.24585555 | 4.10543833 | 4.95755341 |
| 50 | 0.46889651 | 1.43348553 | 2.35654885 | 3.24599291 | 4.10703835 | 4.94114551 |
| 60 | 0.46889651 | 1.43348555 | 2.35654908 | 3.24598255 | 4.10694346 | 4.94337909 |

TABLE I: Eigenvalues of the PDM $H_1$ for different iteration numbers $k$ and $\gamma = 0.1$.

and $H_4$.Again we have used 60 iterations for each Hamiltonians and checked stability of the eigenvalues. Here we calculated eigenvalues for 30 iterations and they are listed in Table II. We have also checked that for the given eigenvalues, the wave functions are normalizable and it tends to zero when $x \to \infty$.

| $n$ | $E_{H_2}$ | $E_{H_3}$ | $E_{H_4}$ |
|---|---|---|---|
| 0 | 0.50773226 | 0.48833347 | 0.50949336 |
| 1 | 1.45551369 | 1.44451856 | 1.45972923 |
| 2 | 2.36941282 | 2.36286881 | 2.37461896 |
| 3 | 3.25544187 | 3.25137213 | 3.26106459 |
| 4 | 4.13235379 | 4.12882619 | 4.13805287 |
| 5 | 4.95997506 | 4.96305356 | 4.96478901 |

TABLE II: The eigenvalues Hamiltonians $H_2$, $H_3$ and $H_4$, for $\gamma = 0.1$. The result is obtained after 30 iterations.

The results given in Table II shows that eigenvalues and eigenfunctions are also depends on the choices of the parameters, $\varepsilon, \rho$, and $\eta$ of Hamiltonian (9).

## REMARKS AND DISCUSSIONS

In this paper, we have studied the solution of the PDM Schrödinger equation without mapping the potential in to the mass space. We have solved PDM Schrödinger equation for four different kinetic energy operators including harmonic oscillator potential with the variable mass function of the form $m(x) = m_0\,(1 + \gamma x^2)$. It is shown that energy levels

FIG. 1: Plot of the normalized wave function of the PDM Hamiltonian (10a) for $n = 0, 1, 2, 3, 4, 5$.

of the PDM Schrödinger equation depends on the mass distributions. It is important to remark that the results presented here, shows that eigenvalues also depends on the ordering parameters of the PDM Schrödinger equation [72].

We have presented an approximate method based on asymptotic Taylor Series Expansion of a function. Fortunately, this method is useful for obtaining both eigenvalues and eigen-

functions of the Schrödinger type equations. Therefore, the results have been obtained here, allowing further comparisons between the models.

As a further work the method presented here can be used to built more realistic models for the PDM physical systems. Before ending this work a remark is in order. When the potential mapped to the mass space, the both constant and PDM Hamiltonian has the same eigenvalues. It will be worthwhile to discuss physical acceptability of such an isospectrality in the position dependent mass background. Therefore we have to develop methods for solving PDM Schrödinger equation without connecting mass to potential or vice versa.

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