Remarks on the solution of the position-dependent mass Schrödinger equation

Ramazan Koç and Seda Sayın
Faculty of Engineering, Department of Physics, Gaziantep University, 27310 Gaziantep, Turkey
E-mail: koc@gantep.edu.tr and ssayin@gantep.edu.tr

Received 27 May 2010, in final form 1 September 2010
Published 19 October 2010
Online at stacks.iop.org/JPhysA/43/455203

Abstract
An approximate method is proposed to solve the position-dependent mass (PDM) 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 versa. The method based on the 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 the 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.

PACS numbers: 03.65.Ge, 03.65.Fd, 02.30.–f

1. 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 and developing theoretical models for effective interactions in nuclear physics, neutron stars, liquid crystals and metal clusters [1–15]. These applications have stimulated a naturally renewed interest in the solution of PDM quantum mechanical Hamiltonians. Recently, the solutions of the PDM Schrödinger equation, the Dirac equation [16–19] and the Klein–Gordon equation [20–22] have received much attention. A number of authors have studied the 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, the PDM Schrödinger equation has been transformed in the form of the constant mass Schrödinger equation by changing coordinate and wavefunction. 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 the coordinate and wavefunction becomes a bridge between the constant mass and PDM Schrödinger equation. As an example in a constant mass Schrödinger equation the choice of coordinate $u = \int_0^x \sqrt{m(x)} \, dx$ and wavefunction $\psi(u) = [2m(x)]^{1/4} \varphi(x)$ provides its transformation in the form of the PDM Schrödinger equation. In this case the potential is mass dependent, i.e. the harmonic oscillator potential can be expressed as $V = \frac{1}{2} m \omega^2 u^2 = \frac{1}{2} m \omega^2 \left( \int_0^x \sqrt{m(x)} \, dx \right)^2$ and both the 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 PDM background. In some papers [9–12, 21, 47, 53, 57, 61], the solution of the PDM Schrödinger equation has been obtained without transforming the potential into the mass space. In this case the energy spectrum of the PDM Hamiltonians is not isospectral with the constant mass Hamiltonians. Therefore it is reasonable to develop a method for solving the 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 paper, 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 the PDM Hamiltonian.

It is well known that the study of the same mathematical problems from a different point of view leads 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 the Schrödinger equation which improves both analytical and numerical determination of the eigenvalues. The 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 the wavefunction 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 the construction of the ATEM by reformulating the well-known Taylor series expansion of a function that satisfies the 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 the solution of the PDM Schrödinger equation including the harmonic oscillator potential and the variable mass $m(x) = m_0(1 + \gamma x^2)$ [11]. In this section, we present an approximate analytical expression for the 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.

2. Formalism of the ATEM

In this section, we show the solution of the Schrödinger-type equation for a quite ample class of potentials, by modifying the Taylor series expansion by means of a finite sequence instead of an infinite sequence and its termination possessing the property of the quantum mechanical
wavefunction. Let us consider the Taylor series expansion \([66]\) of a function \(f(x)\) about the point \(a\):

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

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 \(a\). The expansion of the function \(f(x)\) about the origin \((a=0)\) is known as Maclaurin’s series and it is given by

\[
f(x) = f(0) + xf'(0) + \frac{1}{2}x^2 f''(0) + \frac{1}{6}x^3 f'''(0) + \cdots
\]

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

\[
f''(x) = p_0(x)f'(x) + q_0(x)f(x).
\]

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

\[
f^{(n+2)}(x) = p_n(x)f'(x) + q_n(x)f(x),
\]

where

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

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

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

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

After all, we have obtained useful formalism of the Taylor expansion method. In the solution of the eigenvalue problems, truncation of the asymptotic expansion to a finite number of terms is useful. If the series is optimally truncated at the smallest term, then the asymptotic expansion of the series is known as supersymptotic \([71]\), 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 \(x\) is collected as coefficients of \(f(0)\) or \(f'(0)\) and vice versa, the series is truncated at \(n = m\) then there is an immediate practical consequence of these conditions for \(q_{m-2}(0) = 0\) or \(p_{m-2}(0) = 0\). In this way, one of the parameters in \(q_{m-2}(0)\) and/or \(p_{m-2}(0)\) belongs to the spectrum of the Schrödinger equation. Therefore, the 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 the eigenfunction of the system is discrete. Therefore in order to terminate the eigenfunction \(f(x)\) we can concisely write that

\[
q_m(0)f(0) + p_m(0)f'(0) = 0
\]  

\[
q_{m-1}(0)f(0) + p_{m-1}(0)f'(0) = 0;
\]
eliminating \( f(0) \) and \( f'(0) \) we obtain

\[
q_m(0)p_{m-1}(0) - p_m(0)q_{m-1}(0) = 0,
\]

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

In the 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 deal 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 wavefunction.

The process presented here is iterative and the 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 \( m = 40 \), and so on; next we compare the values of the parameter (eigenvalue) in each case till ten digits. If the values of the parameter reach their asymptotic values, then we use these values and omit the others. For instance, if one can obtain the values of the parameters for \( m = 40 \), first few of them will reach their asymptotic values, say first eight values. The following comment on the function is considerable: for such a solution it is suitable to take sum of the first eight terms in (6).

It will be shown that the 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 the PDM Schrödinger equation including large class of potentials of practical interest.

3. Solution of the PDM Schrödinger equation by using the ATEM

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

\[
H = \frac{1}{4}(m^p m^p + m^q m^q + m^p m^q) + V(x),
\]

where \( \eta + \varepsilon + \rho = -1 \) is a constraint and \( m = m(x) \) is the PDM. 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]:

\[
H_1 = \frac{1}{2} \left( \frac{p - p}{m} \right) + V(x) \quad \text{for} \quad \varepsilon = -1, \quad \rho = 0, \quad \eta = 0,
\]

\[
H_2 = \frac{1}{4} \left( \frac{1}{m^p} + \frac{1}{m^q} \right) + V(x) \quad \text{for} \quad \varepsilon = 0, \quad \rho = 0, \quad \eta = -1,
\]

\[
H_3 = \frac{1}{2} \left( \frac{1}{\sqrt{m}^p} + \frac{1}{\sqrt{m}^q} \right) + V(x) \quad \text{for} \quad \varepsilon = -\frac{1}{2}, \quad \rho = 0, \quad \eta = -\frac{1}{2},
\]

\[
H_4 = \frac{1}{2} \left( \frac{p - p}{\sqrt{m}^p} + \frac{p - p}{\sqrt{m}^q} \right) + V(x) \quad \text{for} \quad \varepsilon = 0, \quad \rho = -\frac{1}{2}, \quad \eta = -\frac{1}{2}.
\]

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

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

\[ H_{\gamma} \psi(x) = E \psi(x) \quad (i = 1, 2, 3, 4), \tag{11} \]

including the harmonic oscillator potential, \( V(x) = \frac{1}{2} m \omega^2 x^2 \), we use the mass distributions \( m(x) = m_0 (1 + \gamma x^2) \), where \( \gamma \) is arbitrary positive constant. By the way, we emphasize that the wavefunction of the harmonic oscillator potential is well defined in the region of \( \pm \infty \) and satisfy that \( \lim_{x \to \pm \infty} |\psi(x)|^2 \to 0 \). In this limit the mass distributions are to be continuous.

It is well known that the asymptotic behavior of the constant mass Schrödinger equation including the 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 the wavefunction guarantees \( \lim_{x \to \pm \infty} \frac{|\psi(x)|^2}{\sqrt{m}} \to 0 \). 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.

### 3.1. Asymptotic analysis

The term asymptotic means the function approaching to a given value as the iteration number tends to infinity. With the help of a Mathematica program we calculate eigenvalues and eigenfunction of \( H_{\gamma} \) for \( \gamma = 0.1 \) using the number of iterations \( k \) = [20, 30, 40, 50, 60]. The function \( f(x) \) for the \( n = 2 \) state is given in (12) and eigenvalues are presented in table 1:

| \( k \) | \( n = 0 \) | \( n = 1 \) | \( n = 2 \) | \( n = 3 \) | \( n = 4 \) | \( n = 5 \) |
|---|---|---|---|---|---|---|
| 20 | 0.468 890 47 | 1.433 412 11 | 2.357 655 42 | 3.283 974 86 | 4.213 603 62 | 4.353 995 96 |
| 30 | 0.468 896 65 | 1.433 480 58 | 2.356 422 59 | 3.246 608 34 | 4.120 869 16 | 4.983 213 27 |
| 40 | 0.468 896 50 | 1.433 485 82 | 2.356 555 07 | 3.245 855 55 | 4.105 438 33 | 4.957 553 41 |
| 50 | 0.468 896 51 | 1.433 485 53 | 2.356 548 85 | 3.245 992 91 | 4.107 038 35 | 4.941 145 51 |
| 60 | 0.468 896 51 | 1.433 485 55 | 2.356 549 08 | 3.245 982 55 | 4.106 943 46 | 4.943 379 09 |

Our calculation gives an accurate result for first eight eigenvalues and eigenfunctions after 40 iterations. Here we have used 60 iterations. Figure 1 shows the plot of normalized wavefunctions for first six states.

#### 3.1.1. Solution of the Hamiltonians \( H_2 \), \( H_3 \) and \( H_4 \)

In the previous section we have illustrated applicability of our method by solving the Hamiltonian \( H_1 \). In this section we apply the same procedure to solve the Hamiltonians \( H_2 \), \( H_3 \) and \( H_4 \). Again we have used 60 iterations for each Hamiltonian and checked the stability of the eigenvalues. Here we calculated eigenvalues for
Figure 1. Plot of the normalized wavefunction of the PDM Hamiltonian (10a) for \( n = 0, 1, 2, 3, 4, 5 \).

30 iterations and they are listed in table 2. We have also checked that for the given eigenvalues, the wavefunctions are normalizable and it tends to zero when \( x \to \infty \).

The results given in table 2 show that eigenvalues and eigenfunctions also depend on the choices of the parameters \( \epsilon, \rho \) and \( \eta \) of the Hamiltonian (9).

4. Remarks and discussions

In this paper, we have studied the solution of the PDM Schrödinger equation without mapping the potential into the mass space. We have solved the PDM Schrödinger equation for four different kinetic energy operators including the 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 of the PDM Schrödinger equation depends on the mass distributions. It is important to remark that the
results presented here shows that eigenvalues also depend on the ordering parameters of the PDM Schrödinger equation [72].

We have presented an approximate method based on the asymptotic Taylor series expansion of a function. Fortunately, this method is useful for obtaining both eigenvalues and eigenfunctions 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 is mapped to the mass space, the both constant and the PDM Hamiltonian has the same eigenvalues. It will be worthwhile to discuss physical acceptability of such an isospectrality in the PDM background. Therefore, we have to develop methods for solving the PDM Schrödinger equation without connecting mass to potential or vice versa.

Acknowledgment

The research was supported by the Scientific and Technological Research Council of TURKEY (TÜBİTAK).

References

[1] Serra L I and Lipparini E 1997 Europhys. Lett. 40 667
[2] Barranco M, Pi M, Gatica S M, Hernandez E S and Navarro J 1997 Phys. Rev. B 56 8997
[3] Bastard G 1988 Wave Mechanics Applied to Semiconductor Heterostructure (Les Ulis: Editions de Physique)
[4] Köç R, Koca M and Sahinoglu G 2005 Eur. Phys. J. B 48 583
[5] Geller M R and Kohn W 1993 Phys. Rev. Lett. 70 3103
[6] Arias de Saavedra F, Boronat J, Polls A and Fabrocini A 1994 Phys. Rev. B 50 4248
[7] Harrison P 2000 Quantum Wells, Wires and Dots (New York: Wiley)
[8] Weisbuch C and Vinter B 1993 Quantum Semiconductor Heterostructure (New York: Academic)
[9] Peter A J and Naraneethakrishnan K 2008 Physica E 40 2747
[10] Khordad R 2010 Physica E 42 1503
[11] Schmidt A G M, Azeredo A D and Gusso A 2008 Phys. Lett. A 372 2774
[12] Ando T and Ohtake Y 2006 Phys. Rev. E 73 066702
[13] Fu Y and Chao K A 1989 Phys. Rev. B 40 8349
[14] Young K 1989 Phys. Rev. B 39 13434
[15] von Roos O and Mavromatis H 1985 Phys. Rev. B 31 2294
[16] Alhaidari A D 2004 Phys. Lett. A 322 72
[17] Roy B 2006 Mod. Phys. Lett. B 20 1033
[18] Ikhdair S M 2010 J. Math. Phys. 51 023525
[19] Peng X L, Liu J Y and Jia C S 2006 Phys. Lett. A 352 478
[20] Ikhdair S M 2009 Eur. Phys. J. A 40 143
