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Variable Mass Quantum Harmonic Oscillator; Exact Solvability and Isospectral Potentials

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Abstract

By imposing a particular constraint of solvability on the Liouville normal form of the BenDaniel-Duke type variable mass Schrödinger equation, we have derived a class of solvable potentials and harmonic oscillator type solutions for the system. The method has been shown to be applicable in finding isospectral potentials for an infinite possibility of position-dependent mass distributions as well as in determining the effective mass profile for a given effective interaction.

Keywords: Variable mass; isospectral potentials; quantum harmonic oscillator; Sturm-Liouville transformation; quantum states; energy spectrum

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1 Introduction

Lately, there has been a flurry of studies on the quantum system with position dependent effective mass (PDEM). Amongst others, one notes: the displacement operator approach [1, 2, 3], application of Meijer *G*-functions for analytic solutions [4, 5], scattering and transport properties at heterojunctions [6, 7], the PDEM system beyond one dimension [8, 9], Solutions in the background of physical potentials [10, 11] and PDEM harmonic oscillators [12, 13]. This field has been on the rise due to the impressive development of sophisticated technologies in the fabrication of ultra thin semiconductor structures with very prominent quantum effects [14, 15]. Position-dependent effective mass Schrödinger equations play an important role in the study of electronic properties of semiconductors, inhomogeneous crystals [16], quantum dots [17] and quantum liquids [18]. Exact solutions of effective mass Schrödinger equations are difficult to obtain, as such, one often resorts to numerical techniques. Certain potentials however allow for exact solutions [18, 19]. Many authors have devoted kin interest to finding exactly solvable potentials for such systems [20, 21, 22], as well as quasi-exactly solvable potentials [23].

The present work has a double objective. Firstly, we wish to contribute to finding general solutions to effective mass Schrödinger equations and secondly to derive a class of potentials that guarantee exact solvability of the one-dimensional variable mass Schrödinger equation.

This work is organized as follows: We give a brief review on the general kinetic energy operator for variable mass systems in section 2. In section 3, we apply the Sturm-Liouville transform to the effective mass equation to obtain one of constant mass which is solved in section 4 for the energy eigen values and wave functions. Comments on the results are made in section 5 and we close with conclusions in section 6.

2 Kinetic Energy Operator for the Effective Mass Schrödinger Equation

It is well known from elementary quantum mechanics that the relative ordering of two non-commuting operators is very important. Defining the kinetic energy operator for a system with position dependent mass is crucial due to the non-commutativity of the momentum and the effective mass. It is necessary that the choice of ordering ensures hermiticity of the kinetic energy operator. The generalized form of the kinetic energy operator for PDEM model first suggested by [24] is as follows:

$$\hat{T} = \frac{1}{4}\left(m^{\mu}\mathbf{p}m^{\sigma}\mathbf{p}m^{\delta} + m^{\delta}\mathbf{p}m^{\sigma}\mathbf{p}m^{\mu}\right) \tag{2.1}$$

$m = m(x)$ is the position-dependent mass and $\mathbf{p}$ the momentum operator. The constants μ, σ and δ known as the von Roos ambiguity parameters are arbitrarily chosen but are governed by the relation: $\mu + \sigma + \delta = -1$. It can be easily verified that the kinetic energy operator $\hat{T}$ is Hermitian [25]. Some variants of $\hat{T}$ are as follows:

$$\hat{T} = \frac{1}{2}\left[\mathbf{p}\frac{1}{m}\mathbf{p}\right] \qquad (\mu = \delta = 0, \sigma = -1) \tag{2.2}$$

$$\hat{T} = \frac{1}{2}\left[\frac{1}{\sqrt{m}}p^2\frac{1}{\sqrt{m}}\right] \qquad (\mu = \delta = \frac{-1}{2}, \sigma = 0) \tag{2.3}$$

$$\hat{T} = \frac{1}{4}\left[\frac{1}{m}p^2 + p^2\frac{1}{m}\right] \qquad (\mu = -1, \sigma = \delta = 0) \tag{2.4}$$

Proposed in [26] , [27] and [28] Respectively.

3 Sturm-Liouville Transformation of the Position-dependent Effective Mass Schrödinger Equation

We shall consider eq. (2.2) for which the following Schrödinger equation is obtained.

$$-\frac{1}{2}\frac{\mathrm{d}}{\mathrm{d}x}\frac{1}{m(x)}\frac{\mathrm{d}}{\mathrm{d}x}\Psi(x)+V(x)\Psi(x)=E_n\Psi(x) \tag{3.1}$$

The wave function $\Psi(x)$ should be continuous at the mass discontinuity and the derivative of the wave function should satisfy the following condition

$$\frac{1}{m(x)}\frac{\mathrm{d}}{\mathrm{d}x}\Psi(x)|_{-}=\frac{1}{m(x)}\frac{\mathrm{d}}{\mathrm{d}x}\Psi(x)|_{+} \tag{3.2}$$

The main concern in solving eq.(3.1) is to obtain the energy spectrum and/or wave functions once the PDEM function is given. However, exact resolvability requirements result in constraints on the potential function $V(x)$ for the given mass distribution. Finding solvable potentials for eq.(3.1) is therefore important.

By performing the transformation:

$$\Psi(x)=\frac{1}{m(x)}\phi(x) \tag{3.3}$$

Equation eq. (3.1) takes the form:

$$-\frac{\mathrm{d}^2\phi(x)}{\mathrm{d}x^2}+3\frac{m'(x)}{m(x)}\frac{\mathrm{d}\phi(x)}{\mathrm{d}x}+U(x)\phi(x)=2E_n m(x)\phi(x) \tag{3.4}$$

Where

$$U(x)=\left[\frac{m''(x)}{m(x)}-3\frac{m'(x)^2}{m(x)^2}+2m(x)V(x)\right] \tag{3.5}$$

Let

$$p(x)=m(x)^{-3} \tag{3.6}$$

Such that:

$$\frac{p'(x)}{p(x)}=-3\frac{m'(x)}{m(x)} \tag{3.7}$$

Substituting in eq. (3.4) we obtain;

$$\frac{\mathrm{d}^2\phi(x)}{\mathrm{d}x^2}+\frac{p'(x)}{p(x)}\frac{\mathrm{d}\phi(x)}{\mathrm{d}x}+\frac{1}{p(x)}\left[q(x)-\lambda\rho(x)\right]\phi(x)=0 \tag{3.8}$$

The quantities in eq. (3.8) have the following definitions:

$$\begin{aligned} q(x) &= -m(x)^{-3}U(x) \\ \rho(x) &= m(x)^{-2} \\ \lambda &= 2E_n \end{aligned} \tag{3.9}$$

Eq. (3.8) is in the Sturm-Liouville form. To transform it into the Liouville normal form, the next three equations are used.

$$
\begin{aligned}
r(x) &= \int_0^x \sqrt{\frac{\rho(s)}{p(s)}}\mathrm{d}s \\
&= \int_0^x \sqrt{m(s)}\mathrm{d}s
\end{aligned} \tag{3.10}
$$

$$
\begin{aligned}
W(r(x)) &= \sqrt[4]{\rho(x)p(x)}\phi(x) \\
&= m(x)^{-5/4}\phi(x)
\end{aligned} \tag{3.11}
$$

$$
\begin{aligned}
Q(r(x)) &= \frac{1}{\rho}\left[-q-(p\rho)^{1/4}\left(p\left(\frac{1}{(p\rho)^{1/4}}\right)'\right)'\right] \\
&= m(x)^2 \\
&\times\left[\frac{U(x)}{m(x)^3}-\frac{1}{m(x)^{5/4}}\left(m(x)^{-3}\left(m(x)^{5/4}\right)'\right)'\right] \\
&= 2V(x)+\frac{7m'(x)^2}{16m(x)^3}-\frac{m''(x)}{4m(x)^2}
\end{aligned} \tag{3.12}
$$

Here, the primes represent differentiation with respect to x. With eq. (3.10),eq. (3.11) and eq. (3.12), eq. (3.8) is transformed to:

$$
-\frac{\mathrm{d}^2W(r)}{\mathrm{d}r^2}+\left[Q(r(x))-\lambda\right]W(r)=0 \tag{3.13}
$$

Eq. (3.13) is in the Liouville normal form. It represents a target system of constant mass equivalent to the initial system eq. (3.1) . Here, $Q(r)$ is the effective potential of the target system. Exact analytic solutions to eq. (3.13) can be obtained for some forms of $Q(r)$. Eq. (3.13) has been derived and solved through different techniques such as: The Darboux transform method [29, 30], super symmetric quantum mechanical approach [31, 32] and the point canonical transformation method [33, 34].

4 Energy Spectrum and Eigen Functions

Using the ansatz

$$
W(r)=\frac{G(r)}{f(r)} \tag{4.1}
$$

Where $f(r)$ is an arbitrary function to be determined later, eq. (3.13) is transformed to:

$$
\frac{\mathrm{d}^2G(r)}{\mathrm{d}r^2}-2\frac{f'(r)}{f(r)}\frac{\mathrm{d}G(r)}{\mathrm{d}r}+\left[\lambda-Q(r)+2\frac{f'(r)^2}{f(r)^2}-\frac{f''(r)}{f(r)}\right] \tag{4.2}
$$

Chosing $f(r)$ in the form:

$$
f(r)=\exp\left(\frac{dr^2}{2}\right) \tag{4.3}
$$

with d an arbitrary constant, eq. (4.2) reduces to;

$$\frac{\mathrm{d}^2G(r)}{\mathrm{d}r^2} - 2dr\frac{\mathrm{d}G(r)}{\mathrm{d}r} + \left[\lambda - Q(r) + d^2r^2 - d\right]G(r) \tag{4.4}$$

The following solvability condition naturally emerges from eq. (4.4):

$$Q(r) - dr^2 = 0 \tag{4.5}$$

By setting

$$\frac{\lambda - d}{2d} = n \tag{4.6}$$

Eq. (4.4) is solved by the Hermite polynomials $H_n\left[\sqrt{d}r\right]$:

$$G(r) = H_n\left[\sqrt{d}r\right] \tag{4.7}$$

4.1 Wave function

Putting eq. (4.7) and eq. (4.3) in eq. (4.1), we have:

$$W_n(r) = A_n \exp\left(-\frac{dr^2}{2}\right)H_n\left[\sqrt{d}r\right] \tag{4.8}$$

The normalization constant A_n is given by:

$$A_n = \frac{1}{\sqrt{2^n\sqrt{\pi}n!}} \tag{4.9}$$

Substituting eq. (4.9) in eq. (3.11), we have:

$$\phi_n(x) = m(x)^{5/4}\exp\left(\frac{-dr^2}{2}\right)H_n\left[\sqrt{d}r\right] \tag{4.10}$$

Finally, substituting eq. (4.10) in eq. (3.3), the solution to eq. (3.1) is obtained thus:

$$\Psi_n(x) = m(x)^{1/4}\exp\left(\frac{-dr^2}{2}\right)H_n\left[\sqrt{d}r\right] \tag{4.11}$$

This is the form obtained for the quantum states of the variable mass quantum harmonic oscillator in [29] through the super symmetric quantum mechanical approach.

4.2 Energy Spectrum

Substituting eq. (3.9) in eq. (4.6), the energy eigenstates are obtained as follows:

$$E_n = d\left(n + \frac{1}{2}\right) \tag{4.12}$$

The spectrum is similar to that of a quantum harmonic oscillator. This is result obtained in [35] through the analytic transfer matrix method. eq. (4.11) and eq. (4.12) agree with [31] where the point canonical transformation method is used.

5 Results and Discussions

To find the form to which $V(x)$ must be constrained in order to yield exact analytic solutions to eq. (3.1), we start by substituting eq. (3.10) in eq. (4.5) such that:

$$Q(r(x)) = d\left[\int_0^x \sqrt{m(s)}\mathrm{d}s\right]^2 \tag{5.1}$$

Substituting eq. (5.1) in eq. (3.12), we arrive at the following class of solvable potentials for the effective mass Schrödinger equation eq. (3.1)

$$V(x) = \frac{d}{2}\left[\int_0^x \sqrt{m(s)}\mathrm{d}s\right]^2 - \frac{7m'(x)^2}{32m(x)^3} + \frac{m''(x)}{8m(x)^2} \tag{5.2}$$

For an illustration, let's consider eq. (5.2) in the case of constant mass:

$$m(0) \equiv m_0 \tag{5.3}$$

In this case, the solvable potential takes the harmonic form:

$$V(x) = \frac{1}{2}dm_0x^2 \tag{5.4}$$

This implies that the starting point for this class of solvable models is the standard quantum harmonic oscillator.

On the other hand, a solution to eq. (5.2) for a given background potential $V(x)$, should yield the mass profile for which eq. (3.1) has solutions of the form; eq. (4.11) and eq. (4.12). Numerical solutions to eq. (5.2) for four different types of potentials are shown in Figure 1.

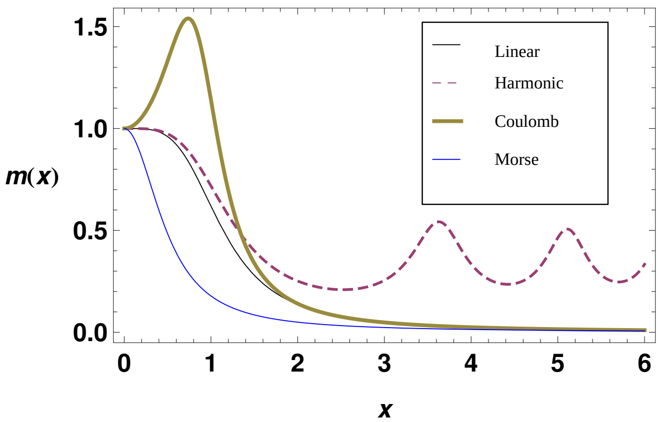

Figure 1: Plot of the mass profile against position probed in the background of the bare potential $V(x)$, with $\gamma = d = 1$

It can be seen from Figure 1 that the harmonic potential does not yield a straight line as one should expect. This signals the onset of a quantum effect which we will state as follows: Once the mass of a quantum system depends on position, the bare background in which it is found experiences a re-shape: $(V(x) \longrightarrow Q(x))$. Let's consider the following definition:

$$\frac{1}{2}Q(x) = V(x) + U_{SA}(x) \tag{5.5}$$

With $U_{SA}(x)$ a term which we shall call the "Self-Action Potential", given by:

$$U_{SA}(x) = \frac{7m'(x)^2}{32m(x)^3} - \frac{m''(x)}{8m(x)^2} \tag{5.6}$$

This is the potential the particle induces on itself as a result of its varying mass. To prob the mass of a quantum system taking into account the quantum effect, we return to eq. (5.1). Results for four types of interactions are shown in Figure 2.

Figures 1 and 2 were simulated using the following functions:

$$\begin{aligned}
\text{Linear potential:} &\quad = \quad \gamma\,(x+1) \\
\text{Harmonic potential:} &\quad = \quad \frac{\gamma}{4}x^2 \\
\text{Coulomb potential:} &\quad = \quad \frac{\gamma}{\gamma + x} \\
\text{Morse potential:} &\quad = \quad \gamma\left(1 + \mathrm{e}^{-2\gamma x}\right)^2
\end{aligned}$$

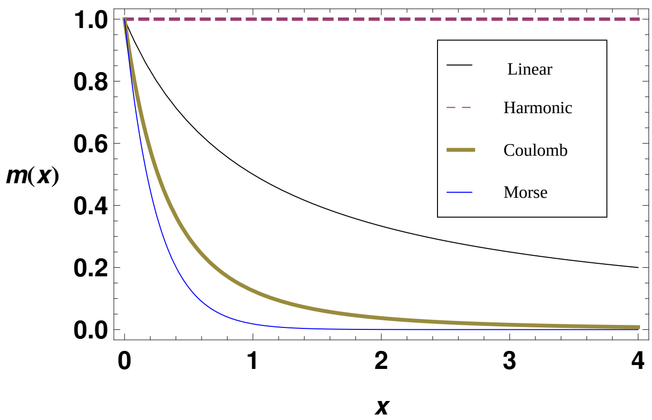

Figure 2: Plot of the mass profile against position with self-action potential taken into account for four cases of the effective interaction $Q(x)$. $\gamma = d = 1$ was used.

It is worth noting that effective mass functions of the form (with b and c arbitrary constants):

$$m(x) = \frac{m_0}{(bx+c)^{4/3}} \tag{5.7}$$

result in a null self-action potential while those of the form used in [1]:

$$m(x) = \frac{m_0}{(bx+c)^2} \tag{5.8}$$

yield a constant self-action potential.

5.1 Applications

We will now construct target solvable systems for some effective mass functions.

5.1.1 Case 1: Quadratic mass function

First we choose a simple quadratic function for the effective mass, i.e.:

$$m(x) = m_0 + \alpha x^2 \tag{5.9}$$

m_0 and α are positive constants. In this case the energy spectrum is obtained from eq. (4.12) and the potential energy and the wave functions are obtained from eq. (5.2) and eq. (4.11) respectively as follows:

$$V(x) = \frac{d}{2}\left(m_0 x + \frac{\alpha x^3}{3}\right)^2 - \frac{7\alpha^2 x^2}{4\,(m_0 + \alpha x^2)^3} + \frac{\alpha}{4\,(m_0 + \alpha x^2)^2} \tag{5.10}$$

$$\Psi_n(x) = A_n\left(m_0 + \alpha x^2\right)^{1/4} \times \exp\left[\frac{-d}{2}\left(m_0 x + \frac{\alpha x^3}{3}\right)^2\right] \times H_n\left[\sqrt{d}\left(m_0 x + \frac{\alpha x^3}{3}\right)\right] \tag{5.11}$$

Figure 3 shows a plot of the probability density function from eq. (5.11).

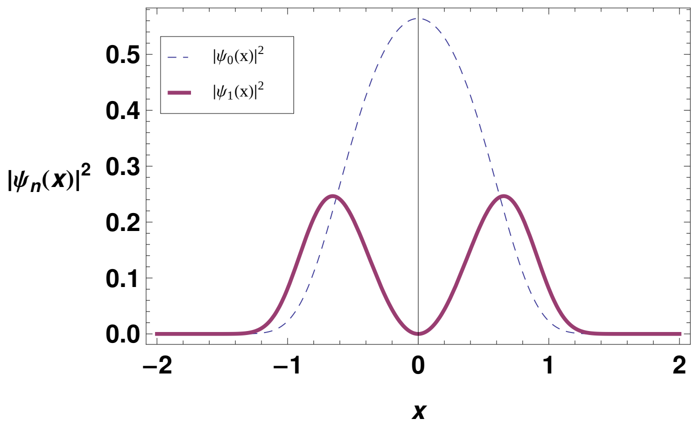

Figure 3: Plot of the density function from eq.(5.11). We used $d = m_0 = \alpha = 1$

5.1.2 Case 2: Asymptotically vanishing mass function

The second form of $m(x)$ is chosen as follows:

$$m(x) = \frac{m_0}{x^2 + \alpha^2} \tag{5.12}$$

In this case, we obtain the following expressions for the potential and the wave functions:

$$V(x) = \frac{dm_0^2}{2\alpha^2}\left[\tan^{-1}\left(\frac{x}{\alpha}\right)\right]^2 - \frac{(\alpha^2+4x^2)}{4m_0(\alpha^2+x^2)} \tag{5.13}$$

$$\begin{aligned} \Psi_n(x) = \quad & A_n\left(\frac{m_0}{\alpha^2+x^2}\right)^{1/4} \\ & \times \exp\left[-\frac{dm_0^2}{2\alpha^2}\tan^{-1}\left(\frac{x}{\alpha}\right)^2\right] \\ & \times H_n\left[\frac{\sqrt{d}m_0}{\alpha}\tan^{-1}\left(\frac{x}{\alpha}\right)\right] \end{aligned} \tag{5.14}$$

Figure 4 shows a plot of the probability density function for the first two states of eq. (5.14)

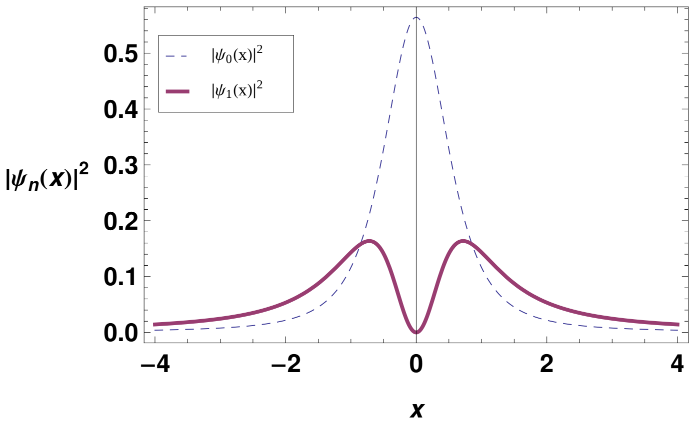

Figure 4: Plot of the density function from eq.(5.14). We used $d = m_0 = \alpha = 1$

5.1.3 Case 3: Hyperbolic mass function

Here we consider a mass function of the form:

$$m(x) = \tanh(ax)^2 \tag{5.15}$$

The Solvable potential is obtained as:

$$\begin{aligned} V(x) = \quad & \frac{dm_0^2}{2\alpha^2}\left[\tanh(\alpha x) - \alpha x\right]^2 \\ & -\frac{\alpha^2}{2m_0}\csc(ax)^2 + \frac{\alpha^2}{4m_0}\csc(ax)^4 \\ & -\frac{7\alpha^2\left(x^2+\alpha^2\right)^3}{4m_0}\sec(\alpha x)^4\tanh(\alpha x)^2 \end{aligned} \tag{5.16}$$

Corresponding wave functions take the for:

$$\begin{aligned}\psi_n(x) = \quad & A_n \left(m_0 \tanh^2(\alpha x)\right)^{1/4} \\ & \times \exp\left[\frac{-d}{2} m_0^2 \left(x - \frac{\tanh(\alpha x)}{\alpha}\right)^2\right] \\ & \times H_n \left[\sqrt{d} m_0 \left(x - \frac{\tanh(\alpha x)}{\alpha}\right)\right] \end{aligned} \tag{5.17}$$

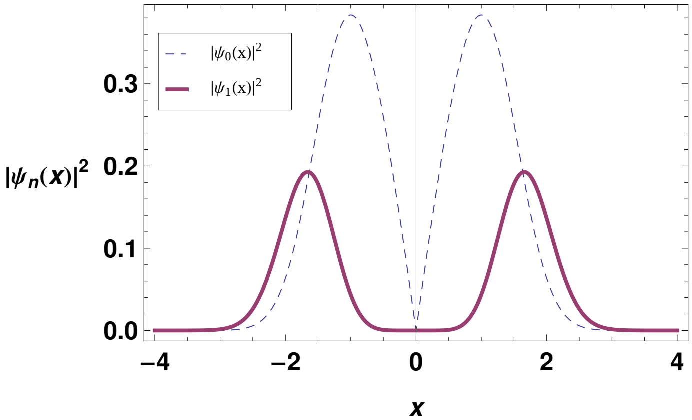

Figure 5: Plot of the density function from eq.(5.17). We used $d = m_0 = \alpha = 1$

6 Conclusions

We have applied the Sturm-Liouville transformation to the BenDaniel-Duke form of the variable mass Schrödinger equation and determined its condition of resolvability. Our solutions, namely; the energy spectrum and wave functions, agree with results obtained through other techniques. Our resolvability constraint eq. (4.5) yields a direct relation between the background potential $V(x)$ and the effective mass $m(x)$. This has allowed us to define a class of solvable potentials eq. (5.2) for the effective mass Schrödinger equation eq. (3.1)

In this approach, there are countless numbers of choices for $m(x)$ for which the wave function and the energy spectra can be obtained in an exact manner. The solution to eq. (5.2) for a given potential should define the variable mass for the system in question. It has been straight forward to observe from eq. (5.2) the prominence of a quantum effect which we have named "self-action potential". This opens a new perspective as to the effect of ordering ambiguity on the self-action potential. At this point, we can state that the initially stated objectives have been met.

we believe that the present approach will prove useful in treating realistic situations which now occur in experimental observations with the advent of the quantum technology, especially as concerns probing the spatial variation of the effective mass of a system when it is under a given interaction.

Competing Interests

The authors declare that no competing interests exist.

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