Remarks on exact solvability of quantum systems with spatially varying effective mass

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Within the frame of a novel treatment we make a complete mathematical analysis of exactly solvable one-dimensional quantum systems with non-constant mass, involving their ordering ambiguities. This work extends the results recently reported in the literature and clarifies the relation between physically acceptable effective mass Hamiltonians.

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The study of quantum mechanical systems with position dependent mass has been raised some important conceptual questions, such as the ordering ambiguity of the momentum and mass operators in the kinetic energy term, the boundary conditions at abrupt interfaces characterized by discontinuities in the mass function, etc. Therefore, the form of the effective mass Hamiltonian has been a controversial subject in the literature. In recent years there has been a growing interest in the study of such systems due to the applications in condensed matter physics and other areas involving quantum many body problem. These applications stimulated a lot of work in the literature regarding the development of techniques for the treatment of such systems, for a recent review, see [1-6] and the related references therein. In all these works the main concern is in obtaining the energy spectra and/or wave functions for quantum systems with spatially dependent effective mass. Moreover, exact solvability requirements result in constraints on the potential functions for the given mass distribution. Though there has been a large consensus in favor of BenDaniel and Duke Hamiltonian (BDD) [7] proposed in the literature as an appropriate one, the question of the exact form of the kinetic energy operator is still an open problem for such systems.

Within this context, the present Letter involves an alternative scheme to obtain unambiguously the Schrödinger equation with non-constant particle mass, which makes clear the relationship between the exact solvability of the Schrödinger equation and the ordering ambiguity. The model explored here restricts naturally the possible choices of ordering and provide us a clear comparison between the
solutions of different but physically plausible effective Hamiltonians clarifying the physics behind ambiguity.

To achieve our goal defined above, the recently developed non-perturbative technique [8] is employed within the frame of supersymmetric quantum mechanics [9]. In this unified model, the BDD Hamiltonian is considered as an unperturbed term while modifications due to other effective Hamiltonians are treated as an additional potential in the same framework. This realization is of prime significance in the calculation of physical processes, which so far did not receive adequate attention.

In the following sections the model used through the work is introduced and its applications are presented where the superiority of the present scheme is also discussed.

There are several ways to define the kinetic energy operator when the mass is variable. Since the momentum and mass operators no longer commute, the generalization of the Hamiltonian is not trivial and this kind of physical problem is intrinsically ambiguous. Starting with the von Roos effective mass kinetic energy operator [10], which has the advantage of an inbuilt Hermicity,

\[ H_{vR} = \frac{1}{4} [m^\alpha(\hat{z})\hat{p}\gamma(\hat{z}) + m^\gamma(\hat{z})\hat{p}\gamma(\hat{z}) + m^\gamma(\hat{z})\hat{p}\alpha(\hat{z})] + V(\hat{z}), \]  

(1)

where \( \alpha + \beta + \gamma = -1 \). By the correspondence in wave mechanics \( \hat{p} \rightarrow -i\hbar \frac{d}{dz}, \hat{z} \rightarrow z \) and on setting

\[ m(z) = m_0 M(z), \quad \hbar = 2m_0 = 1, \]  

(2)

where \( M(z) \) is the dimensionless form of the mass function, the effective mass equation can be written in a differential form,

\[ -\frac{d}{dz} \left[ \frac{1}{M(z)} \frac{d\Psi(z)}{dz} \right] + V^{eff}(z)\Psi(z) = E\Psi(z), \]  

(3)

Here, \( V^{eff}(z) \) is termed the effective potential energy whose algebraic form depends on the Hamiltonian employed

\[ V^{eff}(z) = V_0(z) + U_{\alpha\gamma}(z) = V_0(z) - \frac{(\alpha + \gamma)M''}{2M^2} + (\alpha\gamma + \alpha + \gamma)\frac{M'^2}{M^3}, \]  

(4)

in which the first and second derivatives of \( M(z) \) with respect to \( z \) are denoted by \( M' \) and \( M'' \), respectively. The effective potential is the sum of the real potential profile \( V_0(z) \) and the modification \( U_{\alpha\gamma}(z) \) emerged from the location dependence of the effective mass. A different Hamiltonian leads to a different modification term. Some of them are the ones of BDD (\( \alpha = \gamma = 0 \)), Bastard [11] (\( \alpha = -1 \)), Zhu-Kroemer (ZK) [12] (\( \alpha = \gamma = -\frac{1}{2} \)) and Li-Kuhn [13] (\( \beta = \gamma = -\frac{1}{2} \)).

Considering the supersymmetric treatment of effective mass Hamiltonians by Plastino and his co-workers [14]

\[ A\Psi = \frac{1}{\sqrt{M}} \frac{d\Psi}{dz} + W\Psi, \quad A^+\Psi = -\frac{d}{dz} \left( \frac{\Psi}{\sqrt{M}} \right) + W\Psi, \]  

(5)
where $A$ and $A^+$ are linear operators and $W(z)$ is a superpotential, the supersymmetric Hamiltonians are expressed as

$$H_1 = A^+A = -\frac{1}{M} \frac{d^2}{dz^2} - \left( \frac{1}{M} \right)' \frac{d}{dz} + W^2 - \left( \frac{W}{\sqrt{M}} \right)' ,$$

(6)

and

$$H_2 = AA^+ = H_1 + 2W' \sqrt{M} - \left( \frac{1}{\sqrt{M}} \right) \left( \frac{1}{\sqrt{M}} \right)' .$$

(7)

From which, supersymmetric partner potentials are

$$V_{1^SUSY} = W^2 - \left( \frac{W}{\sqrt{M}} \right)' , \quad V_{2^SUSY} = V_{1^SUSY} + 2W' \sqrt{M} - \left( \frac{1}{\sqrt{M}} \right) \left( \frac{1}{\sqrt{M}} \right)' .$$

(8)

At this stage, we use the spirit of recently developed non-perturbative approach [8] by expressing the total wave function as a product,

$$\Psi(z) = \Phi(z) \Theta(z).$$

(9)

In the above equation, $\Phi$ denotes the wave function corresponding to the unperturbed piece of the effective potential in Eq. (4) while $\Theta$ is the moderating function due to the modified term $U_{\alpha\gamma}$ therein.

The use of (9) in (3) yields

$$\frac{1}{M} \left( \frac{\Phi''}{\Phi} + \frac{\Theta''}{\Theta} + 2 \frac{\Phi' \Theta'}{\Phi \Theta} \right) - \frac{M'}{M^2} \left( \frac{\Phi'}{\Phi} + \frac{\Theta'}{\Theta} \right) = V_{eff} - E,$$

(10)

which reduces to the usual Schrödinger equation with a constant mass when $M \rightarrow 1$. With the consideration of (6), where the superpotential now can be given as

$$W(z) = W_0(z) + \Delta W(z),$$

(11)

with $W_0$ and $\Delta W$ being superpotentials corresponding to the unperturbed potential ($V_0$) and modification term ($U_{\alpha\gamma}$) respectively, Eq. (10) is transformed into a couple of equation,

$$W'^2_0 - \left( \frac{W_0}{\sqrt{M}} \right)' = V_0 - E_0, \quad W_0 = -\frac{1}{\sqrt{M}} \frac{\Phi'}{\Phi},$$

(12)

$$\Delta W'^2 - \left( \frac{\Delta W}{\sqrt{M}} \right)' + 2W_0 \Delta W = U_{\alpha\gamma} - \Delta E, \quad \Delta W = -\frac{1}{\sqrt{M}} \frac{\Theta'}{\Theta}.$$  

(13)

In the above equations, $E = E_0 + \Delta E$ due to $V_{eff} = V_0 + U_{\alpha\gamma}$. Therefore one can easily see the contributions, if any, to the energy and wave function due to the use of effective Hamiltonians other than BDD which represents the unperturbed Hamiltonian in the present scenario since it has no modification term, see (4).
We are familiar with (12) as a standard supersymmetric treatment of the Schrödinger equation for the exact solutions. However, Eq. (13) is new and is the most significant piece of the work presented in this letter. Because it is a non-perturbative approach by Riccati equation, which reproduces the whole corrections coming from $U_{\alpha \gamma}$ if, of course, Eq. (13) is exactly solvable.

To proceed we remind a general consensus [5, 13] that the resolution of the ordering ambiguity in this problem could come from a scheme that starts with the relativistic Dirac equation with spatially varying mass then taking the non-relativistic limit. This is due to the fact that the Dirac equation is inherently free from the ordering ambiguity and that taking the non-relativistic limit is a well defined procedure. Bearing in mind this point we propose a correct choice of $\Delta W$ as

$$\Delta W = \left(\frac{\alpha + \gamma}{2}\right) \frac{M'}{M^{3/2}}, \quad (14)$$

which directs us to find correct ordering parameter(s) leading to the physically plausible effective Hamiltonian(s). Through Eq. (13), the parameters get decoupled in a natural way and the ambiguity in the choice of proper kinetic energy operator disappears. Substituting (14) into (13), we obtain

$$\Delta W^2 - \left(\frac{\Delta W}{\sqrt{M}}\right)' = U_{\alpha \gamma}, \quad \Delta E = -2W_0\Delta W, \quad (15)$$

if either $\alpha = \gamma = 0$ which yields the BDD Hamiltonian or $\alpha = \gamma = -\frac{1}{2}$ corresponding to the ZK Hamiltonian. It is stressed that the results are independent of any choice of $M(z)$ and in case $\alpha = \gamma = 0$ Eq. (13) vanishes. This restriction is in agreement with the discussion in Ref. [15] and also with the work of Bagchi et al [3].

Though the present formalism has a wide spread applicability, for clarity we now simply consider the two examples which were investigated in Ref.[14]. This consideration will shed a light in understanding the interrelation between the BDD and ZK effective Hamiltonians bearing in mind the results presented in [14] for the systems of interest.

The simplest case of the shape invariance integrability condition [9], leading to exactly solvable potentials, corresponds a uniform energy shift $\varepsilon$ between partner potentials,

$$V_2^{SUSY}(z, \varepsilon) - V_1^{SUSY}(z, \varepsilon) = \varepsilon = 2E_0 \quad (16)$$

since $\Delta E$ term appearing in the partners due to $U_{\alpha \gamma}$ cancels each other. The replacement of (8) into (16) gives

$$\frac{2(W_0' + \Delta W')}{\sqrt{M}} - \left(\frac{1}{\sqrt{M}}\right)'' = \varepsilon, \quad (17)$$
from which one finds the superpotentials leading to the hamiltonian with $V_0$, 

$$W_0(z) = -\frac{1}{2} \left( \frac{1}{\sqrt{M}} \right) \frac{d}{dz} + \frac{\epsilon}{2} \int^z \sqrt{M(y)} dy,$$  

(18)  

since $\Delta W = -(M'/2M^{3/2}) = \left( \frac{1}{\sqrt{M}} \right)'$. To finalize the full treatment, one needs the total superpotential, $W = W_0 + \Delta W$ from which the results in [14], Eq. (35) and the subsequent equations, can easily be reproduced.  

From this short discussion, it is obvious that (i) there will be no contribution to $E_0$ due to the modification term. For this reason total energies in both system having a constant mass and position dependent mass are equal. (ii) From (13), the contribution of $U_{\alpha\gamma}$ to the unperturbed wave function is (for the ground state) 

$$\Theta_{n=0}(z) = \exp \left(-\int^z \sqrt{M(y)} \Delta W(y) dy \right) = m^{1/2}.  

(19)  

Thus, going back to (9) along with Eqs. (12) and (18), the full unnormalized ground state wave function is expressed as 

$$\Psi_{n=0}(z) = \left[ m^{-1/4}(z) \Phi(\bar{z}) \right] m^{1/2}(z) = m^{-1/4}(z) \Phi(\bar{z}),  

(20)  

where $\bar{z} = \int^z \sqrt{M(y)} dy$, which supports the reliability of the present formalism [1]. The excited state wave functions can be determined [9] in algebraic fashion by successive application of the linear operators in (5) upon the ground state wave function. (iii) The both choice, namely the BDD and ZK Hamiltonians are represented with a unique superpotential leading to exactly equivalent wave functions for shape invariant potentials. (iv) From (8), as $\alpha = \gamma = -\frac{1}{2}$, one gets 

$$V_2^{SUSY} = \left( V_1^{SUSY} + U_{\alpha\gamma} \right) + \frac{2W'}{\sqrt{M}},  

(21)  

pointing a duality between BDD and ZK schemes, which reveals the suggestions in [1, 3].

Let us proceed with another example in Ref. [14] where the superpotential leads to a Morse-like spectra, 

$$W(z, A) = A + f(z),  

(22)  

in which, within the frame of the present formalism, $f(z) = f_0(z) + \Delta f(z)$ that turns the form of (22) into 

$$W(z, A) = [A + f_0(z)] + \Delta f(z) = W_0 + \Delta W(z).  

(23)  

From the shape invariance condition $V_2^{SUSY} (z, A) = V_1^{SUSY} (z, A-\lambda) + R(A)$ used in the supersymmetric quantum theory [9], where $A$ is the potential parameter
and $R$ involving both parameter, $A$ and $\lambda$, leads to the ground state energy of the system. In the light of the work carried out in [14], the substitution of (23) in (8) within the frame of shape invariance condition above produces

$$\frac{2 (f_0' + \Delta f')}{\sqrt{M}} - \frac{1}{\sqrt{M}} \left( \frac{1}{\sqrt{M}} \right)'' = \lambda \left( \frac{1}{\sqrt{M}} \right)' - 2\lambda (f_0 + \Delta f). \quad (24)$$

Remembering $\Delta W = \Delta f = \left( \frac{1}{\sqrt{M}} \right)'$ for $\alpha = \gamma = -\frac{1}{2}$, the above equation is rearranged as

$$f_0'(z) + b_1(z)f_0(z) = b_2(z), \quad (25)$$

where

$$b_1 = \lambda \sqrt{M}, \quad b_2 = - \left[ \frac{\lambda}{2} \sqrt{M} \left( \frac{1}{\sqrt{M}} \right)' + \frac{1}{2} \left( \frac{1}{\sqrt{M}} \right)'' \right]. \quad (26)$$

From (24) it is clear that $\Delta f$ term affects only $b_2$, since when $\Delta f \to 0$ $b_2 \to -b_2$. The solution of differential equation in (25) gives

$$f_0(z) = \left\{ C + \int^z b_2(y) dy \exp \left[ \int^t b_1(t) dt \right] \right\} \times \exp \left[ - \int^z b_1(y) dy \right], \quad (27)$$

where $C$ is an integration constant. Employing the mass function used in [14], $M = [(\alpha + z^2)/(1 + z^2)]^2$, we obtain

$$W(z) = W_0 + \Delta W =$$

$$= \left( A + C \exp \left[ -\lambda \{ z + (\alpha - 1) \arctan x \} \right] - \frac{z(\alpha - 1)}{\alpha + z^2} \right) + 2 \frac{z(\alpha - 1)}{\alpha + z^2}, \quad (28)$$

that is Eq. (53) in [14]. From (12), the corresponding potential function, energy and wave function can be expressed as in [14], which are out of interest in this letter. Generalization of the above discussion to a formalism which is applicable to all spatially varying masses, yields

$$W(z) = W_0 + \Delta W = \left\{ A + C \exp \left[ - \int^z b_1(y) dy \right] - \left( \frac{1}{2 \sqrt{M}} \right)' \right\} + \left( \frac{1}{\sqrt{M}} \right)' \quad (29)$$

Plastino and co-workers [14] studied this problem in case $\alpha = \gamma = 0$ considering only the BDD Hamiltonian and arrived at Eq. (53) in their work, which addresses (28) in our work. This means that BDD and ZK effective Hamiltonians in fact reproduce same results employing an identical superpotential, which once more supports the realization introduced by (21) that they are their supersymmetric partners.

In this work we have discussed the problem of solvability and ordering ambiguity in quantum mechanics for the systems with a position dependent mass.
The present scheme restricts the possible choices of ordering. Proceeding with this consideration it has been observed that the only physically allowable BDD and ZK Hamiltonians are in fact their supersymmetric partners that reproduce identical results in their independent considerations due to use of an identical superpotential. We hope that this observation would make a contribution to the ongoing debate in the literature regarding the isospectral effective mass Hamiltonians.

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References


