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Research Article

Comparison Theorems for the Position-Dependent Mass Schrödinger Equation

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The following comparison rules for the discrete spectrum of the position-dependent mass (PDM) Schrödinger equation are established. (i) If a constant mass m_0 and a PDM $m(\mathbf{x})$ are ordered everywhere, that is either, $m_0 \leq m(\mathbf{x})$ or $m_0 \geq m(\mathbf{x})$, then the corresponding eigenvalues of the constant-mass Hamiltonian and of the PDM Hamiltonian with the same potential and the BenDaniel-Duke ambiguity parameters are ordered. (ii) The corresponding eigenvalues of PDM Hamiltonians with the different sets of ambiguity parameters are ordered if $\nabla^2(1/m(\mathbf{x}))$ has a definite sign. We prove these statements by using the Hellmann-Feynman theorem and offer examples of their application.

1. Introduction

Last few decades, quantum mechanical systems with position-dependent mass (PDM) have received considerable attention. The interest stems mainly from the relevance of the PDM background for describing the physics of compositionally graded crystals [1, 2] and semiconductor nanodevices [3–5]. These applications have stimulated the study of the various theoretical aspects of the PDM Schrödinger equation; in particular, its exact solvability [6–8], shape invariance [9], supersymmetry and intertwining properties [10–12], point canonical transformation [13, 14], iterative solution [15], and relation to theories in curved spaces [16] have been examined.

However, it is known that the PDM Schrödinger equation suffers from ambiguity in operator ordering, caused by the non-vanishing commutator of the momentum operator and the PDM. The PDM Hamiltonians with different ambiguity parameters have been proposed [17–20], but none of them can be preferred according to the existing reliability tests [21–23].

Therefore, the attempts are made to settle the issue by fitting the calculated binding energies to the experimental data [24, 25].

For generelizing such findings and obtaining additional information, one needs some tools to compare the energy eigenvalues predicted by the different PDM Hamiltonians. Within the constant-mass framework, a convenient tool is provided by the so-called comparison theorems [26–28]. For example, the elementary comparison theorem [26, 28] states that if two real potentials are ordered, $V^{(1)} \leq V^{(2)}$, then each corresponding pair of eigenvalues is ordered, $E^{(1)} \leq E^{(2)}$.

The purpose of this paper is to establish the comparison theorems that confront the energy eigenvalues of the constant-mass and PDM Schrödinger equations, as well as the energy eigenvalues of the PDM problems with different ambiguity parameters. Our presentation is based on the Hellmann-Feynman theorem [29, 30] and makes use of the ideas developed for the constant-mass case [28, 31].

The plan of the paper is as follows. In Section 2, we introduce the PDM Hamiltonians and recall the Hellmann-Feynman theorem. In Section 3, the comparison theorems on the PDM background are formulated and proved. In Section 4, we apply these theorems to two PDM problems of current interest. Finally, our conclusions are summarized in Section 5.

2. Preliminaries

For the PDM Schrödinger equation, the most general form of the Hamiltonian is given by [17]

$$H_{\mathrm{pdm}} = -\frac{1}{4}\left(m(\mathbf{x})^{\alpha}\nabla m(\mathbf{x})^{\beta}\nabla m(\mathbf{x})^{\gamma} + m(\mathbf{x})^{\gamma}\nabla m(\mathbf{x})^{\beta}\nabla m(\mathbf{x})^{\alpha}\right) + V(\mathbf{x}), \tag{2.1}$$

where α, β, and γ are the ambiguity parameters ($\alpha + \beta + \gamma = -1$) and the units with $\hbar = 1$ are used. In this paper, we will adopt the sets of the ambiguity parameter values suggested by BenDaniel and Duke [18] ($\alpha = \gamma = 0$, $\beta = -1$), Li and Kuhn [19] ($\alpha = \beta = -1/2$, $\gamma = 0$), and Gora and Williams [20] ($\alpha = -1$, $\beta = \gamma = 0$). Although there are infinitely many alternative values of α, β, and γ constrained by $\alpha+\beta+\gamma = -1$, our derivation of the comparison theorems requires some quantum mean values to have definite signs that imposes further restrictions. As we will see, these amount to choose $\alpha = 0$ or $\gamma = 0$ still capturing most of the ambiguity patameter sets known in literature.

The methods we are going to apply are valid for arbitrary dimension N. We suppose that the Hamiltonian operators have domains $\mathfrak{D}(H) \subset L^2(R^N)$; they are bounded below, essentially self-adjoint, and have at least one discrete eigenvalue at the bottom of the spectrum.

To derive our main results, we need the Hellmann-Feynman theorem [29, 30]. This theorem states that if the Hamiltonian of a system is $H(a)$, where a is a parameter, and the eigenvalue equation for a bound state is $H(a)|a\rangle = E(a)|a\rangle$, where $E(a)$ is the energy and $|a\rangle$ the normalized associated eigenstate, then

$$\frac{\partial E(a)}{\partial a} = \left\langle a\left|\frac{\partial H(a)}{\partial a}\right|a\right\rangle. \tag{2.2}$$

Note that the proof relies on the self-adjointness of $H(a)$ and does not change for PDM Hamiltonians.

3. Comparison Theorems

First, let us formulate the theorem that confronts the energy eigenvalues of the constant mass and BenDaniel-Duke PDM Hamiltonians with the same potentials.

Theorem 3.1. *Suppose that the Hamiltonian*

$$H^{(0)} = -\frac{1}{2m_0}\nabla^2 + V(\mathbf{x}) \tag{3.1}$$

with a real potential $V(\mathbf{x})$ and a constant mass m_0 has discrete eigenvalues $E^{(0)}_{\{n\}}$ characterized by a set of quantum numbers $\{n\}$. Then, the corresponding eigenvalues $E^{(BD)}_{\{n\}}$ of the BenDaniel-Duke PDM Hamiltonian

$$H^{(BD)} = -\frac{1}{2}\nabla\frac{1}{m(\mathbf{x})}\nabla + V(\mathbf{x}) \tag{3.2}$$

satisfy

$$\begin{aligned} E^{(0)}_{\{n\}} &\le E^{(BD)}_{\{n\}} \quad \text{if } \forall \mathbf{x}\ 0 < m(\mathbf{x}) \le m_0, \\ E^{(0)}_{\{n\}} &\ge E^{(BD)}_{\{n\}} \quad \text{if } \forall \mathbf{x}\ m(\mathbf{x}) \ge m_0, \end{aligned} \tag{3.3}$$

provided that these eigenvalues exist.

Proof. Define the Hamiltonian

$$H(a) = (1-a)H^{(0)} + aH^{(\mathrm{BD})}, \tag{3.4}$$

which turns into $H^{(0)}$ and $H^{(\mathrm{BD})}$ when $a = 0$ and $a = 1$, respectively. Assume that $H^{(a)}$ possesses well defined eigenvalues $E_{\{n\}}(a)$, for $0 \le a \le 1$, and the normalized associated eigenfunctions in the coordinate representation are $\psi_{\{n\}}(\mathbf{x}; a)$.

Applying the Hellmann-Feynman theorem (2), we get

$$\frac{\partial E_{\{n\}}(a)}{\partial a} = \int \psi^*_{\{n\}}(\mathbf{x}; a)\left(\frac{1}{2m_0}\nabla^2 - \frac{1}{2}\nabla\frac{1}{m(\mathbf{x})}\nabla\right)\psi_{\{n\}}(\mathbf{x}; a)d\mathbf{x}, \tag{3.5}$$

where the integration is performed over the whole space and the asterisk denotes complex conjugation.

Integrating by parts and taking into account that $\psi_{\{n\}}(\mathbf{x}; a)$ and $\nabla\psi_{\{n\}}(\mathbf{x}; a)$ must vanish at infinity, we obtain

$$\frac{\partial E_{\{n\}}(a)}{\partial a} = \frac{1}{2}\int\left(\frac{1}{m(\mathbf{x})} - \frac{1}{m_0}\right)\left|\nabla\psi_{\{n\}}(\mathbf{x}; a)\right|^2 d\mathbf{x}. \tag{3.6}$$

It is a positive (negative) number if $0 < m(\mathbf{x}) \leq m_0$ ($m(\mathbf{x}) \geq m_0$) for all $\mathbf{x}$, so that $E_{\{n\}}(a)$ is an increasing (decreasing) function of a. For definiteness, let $0 < m(\mathbf{x}) \leq m_0$. Then, it follows immediately that

$$E_{\{n\}}(0) = E_{\{n\}}^{(0)} \leq E_{\{n\}}^{(\mathrm{BD})} = E_{\{n\}}(1) \tag{3.7}$$

that completes the proof. Note that an alternative proof can be given by applying the variational characterization [32] of the discrete part of the Schrödinger spectrum. □

It is now tempting to compare the eigenvalues of the constant-mass Hamiltonian with those of PDM Hamiltonians other than the BenDaniel-Duke one. However, in that case, at least one of the ambiguity parameters α and γ in (2.1) must be nonzero and we encounter an obstacle that becomes clear if we first find out how the eigenvalues of different PDM Hamiltonians are ordered. This is done in the following theorem.

Theorem 3.2. *The discrete eigenvalues $E_{\{n\}}^{(BD)}$, $E_{\{n\}}^{(LK)}$, and $E_{\{n\}}^{(GW)}$ of the BenDaniel-Duke, Li-Kuhn, and Gora-Williams PDM Hamiltonians:*

$$H^{(BD)} = -\frac{1}{2}\nabla\frac{1}{m(\mathbf{x})}\nabla + V(\mathbf{x}), \tag{3.8}$$

$$H^{(LK)} = -\frac{1}{4}\left(\frac{1}{\sqrt{m(\mathbf{x})}}\nabla\frac{1}{\sqrt{m(\mathbf{x})}}\nabla + \nabla\frac{1}{\sqrt{m(\mathbf{x})}}\nabla\frac{1}{\sqrt{m(\mathbf{x})}}\right) + V(\mathbf{x}), \tag{3.9}$$

$$H^{(GW)} = -\frac{1}{4}\left(\frac{1}{m(\mathbf{x})}\nabla^2 + \nabla^2\frac{1}{m(\mathbf{x})}\right) + V(\mathbf{x}) \tag{3.10}$$

satisfy

$$E_{\{n\}}^{(BD)} < E_{\{n\}}^{(LK)} < E_{\{n\}}^{(GW)} \quad \text{if } \forall\mathbf{x}\ \nabla^2\left(\frac{1}{m(\mathbf{x})}\right) < 0, \tag{3.11}$$

$$E_{\{n\}}^{(BD)} > E_{\{n\}}^{(LK)} > E_{\{n\}}^{(GW)} \quad \text{if } \forall\mathbf{x}\ \nabla^2\left(\frac{1}{m(\mathbf{x})}\right) > 0, \tag{3.12}$$

provided that these eigenvalues exist.

Proof. Let us prove the inequalities for $E_{\{n\}}^{(\mathrm{BD})}$ and $E_{\{n\}}^{(\mathrm{LK})}$. We define the parameter-dependent Hamiltonian $H(a)$ by

$$H(a) = (1-a)H^{(\mathrm{BD})} + aH^{(\mathrm{LK})} \tag{3.13}$$

and make use of the Hellmann-Feynman theorem (2.2), to obtain

$$\frac{\partial E_{\{n\}}(a)}{\partial a} = \int \psi^*_{\{n\}}(\mathbf{x};a)\left[\frac{1}{2}\nabla\frac{1}{m(x)}\nabla - \frac{1}{4}\left(\frac{1}{\sqrt{m(\mathbf{x})}}\nabla\frac{1}{\sqrt{m(\mathbf{x})}}\nabla + \nabla\frac{1}{\sqrt{m(\mathbf{x})}}\nabla\frac{1}{\sqrt{m(\mathbf{x})}}\right)\right]\psi_{\{n\}}(\mathbf{x};a)d\mathbf{x}. \tag{3.14}$$

Integration by parts yields

$$\begin{aligned}\frac{\partial E_{\{n\}}(a)}{\partial a} &= -\frac{1}{2}\int \frac{1}{m(\mathbf{x})}\left|\nabla\psi_{\{n\}}(\mathbf{x};a)\right|^2 d\mathbf{x} \\ &\quad + \frac{1}{4}\int \nabla\left(\frac{1}{\sqrt{m(\mathbf{x})}}\psi^*_{\{n\}}(\mathbf{x};a)\right)\cdot\frac{1}{\sqrt{m(\mathbf{x})}}\nabla\psi_{\{n\}}(\mathbf{x};a)d\mathbf{x} \\ &\quad + \frac{1}{4}\int \nabla\left(\frac{1}{\sqrt{m(\mathbf{x})}}\psi_{\{n\}}(\mathbf{x};a)\right)\cdot\frac{1}{\sqrt{m(\mathbf{x})}}\nabla\psi^*_{\{n\}}(\mathbf{x};a)d\mathbf{x} \\ &= -\frac{1}{8}\int \frac{1}{m(\mathbf{x})^2}(\nabla m(\mathbf{x}))\cdot\nabla\left|\psi_{\{n\}}(\mathbf{x};a)\right|^2 d\mathbf{x} \\ &= -\frac{1}{8}\int \nabla^2\left(\frac{1}{m(\mathbf{x})}\right)\left|\psi_{\{n\}}(\mathbf{x};a)\right|^2 d\mathbf{x}.\end{aligned} \tag{3.15}$$

Let $\nabla^2(1/m(\mathbf{x})) \le 0$ for all $\mathbf{x}$, then $E_{\{n\}}(a)$ is an increasing function and we get

$$E_{\{n\}}(0) = E^{(\mathrm{BD})}_{\{n\}} < E^{(\mathrm{LK})}_{\{n\}} = E_{\{n\}}(1) \tag{3.16}$$

that completes the proof. For the case of $E^{(\mathrm{LK})}_{\{n\}}$ and $E^{(\mathrm{GW})}_{\{n\}}$, the proof is identical since the factor $\nabla^2(1/m(\mathbf{x}))$ arises in this case as well. However, it is hardly possible to extend the theorem to the situations when both the ambiguity parameters α and γ are nonzero. The reason is that integrals like (3.15) then contain extra terms (proportional to $\alpha\gamma(\nabla m(\mathbf{x}))^2$), so that the $\nabla^2(1/m(\mathbf{x}))$ term cannot determine the sign by itself. □

Moreover, it is now evident from (3.6) and (3.15) that if we try to compare $E^{(\mathrm{LK})}_{\{n\}}$ with the constant-mass energy $E^{(0)}_{\{n\}}$, then the sign of the integral will be determined by the signs of both $(1/m(\mathbf{x}) - 1/m_0)$ and $\nabla^2(1/m(\mathbf{x}))$. Unfortunately, this leads to inconsistent conditions. For example, in order to get the inequality $E^{(0)}_{\{n\}} > E^{(\mathrm{LK})}_{\{n\}}$, we have to put $1/m(\mathbf{x}) < 1/m_0$ and $\nabla^2(1/m(\mathbf{x})) > 0$; that is, $1/m(\mathbf{x})$ must be bounded from above and convex which is impossible. The same obstacle is encountered when dealing with $E^{(\mathrm{GW})}_{\{n\}}$.

4. Applications

In this section, we consider two specific PDM problems, which are discussed in literature and show how the comparison theorems explain the peculiarities of their energy spectra.

Case 1. The three-dimensional mass distribution of the form

$$m(r) = \frac{m_0}{(1+\kappa r)^2}, \tag{4.1}$$

with $r = |\mathbf{x}|$ and nonnegative κ has been shown [16] to give rise to an exactly solvable extension of the Coulomb problem, $V(r) = -Ze^2/r$. This extension is useful as it enables one to trace the link between the PDM background and theories with deformations in the quantum canonical relations or with curvature of the underlying space.

For this case, the discrete energy eigenvalues of the PDM Hamiltonian (2.1), in units with $\hbar = m_0 = e = 1$, are written as [16]

$$\begin{aligned} E = &-\frac{\left[Z - (\kappa/2)\left(l(l+1) - 2\beta\right)\right]^2}{2n^2} + \frac{Z\kappa}{2} \\ &+ \frac{\kappa^2}{8}\Big[2l(l+1) - n^2 - 4\beta + (1+4\alpha)(1+4\gamma)\Big], \end{aligned} \tag{4.2}$$

where $l = 0, 1, \ldots$ and $n = l+1, l+2, \ldots$ are the orbital and principal quantum numbers, respectively. In contrast to the constant-mass Coulomb problem, the system has only a finite number of discrete levels, so that the allowed values of l and n are restricted by

$$\frac{\kappa}{2}\Big[l(l+1) + n^2 - 2\beta\Big] < Z. \tag{4.3}$$

Such a restriction implies that in presence of the PDM the energy eigenvalues may be closer to continuum and thus larger than the ordinary Coulomb eigenenergies $E^{(0)} = -Z^2/(2n^2)$ calculated with the mass m_0.

It is Theorems 3.1 and 3.2 that permit us to determine how the energy eigenvalues are ordered. Since in (4.1) we have $m(r) \leq m_0$, the eigenvalues of the BenDaniel-Duke PDM Hamiltonian must obey $E^{(\mathrm{BD})} \geq E^{(0)}$, by Theorem 3.1. Since $\nabla^2(1/m(r)) = (\kappa/m_0)(6\kappa + 4/r) > 0$, it follows from Theorem 3.2 that the eigenvalues of the PDM Hamiltonians with different ambiguity parameters are ordered as $E^{(\mathrm{BD})} > E^{(\mathrm{LK})} > E^{(\mathrm{GW})}$.

In order to illustrate these inequalities, we present Figure 1 where we plot the energy for the ground state ($n = 1, l = 0$) and the first radially excited state ($n = 2, l = 0$), as a function of the deforming parameter κ. In Figure 1, the solid lines correspond to the constant-mass case whereas the broken curves represent the PDM cases with different ambiguity parameters. The circles indicate the points at which the bound states disappear according to (4.3). From Figure 1, we see that, for all allowed κ, it holds that $E^{(\mathrm{BD})} \geq E^{(0)}$, as it was proved, and also $E^{(\mathrm{LK})} \geq E^{(0)}$, but we observe both $E^{(\mathrm{GW})} > E^{(0)}$ and $E^{(\mathrm{GW})} < E^{(0)}$ regions. Furthermore, we can see that the second proved inequality, $E^{(\mathrm{BD})} > E^{(\mathrm{LK})} > E^{(\mathrm{GW})}$, is indeed fulfilled.

Case 2. Now, let us consider the one-dimensional mass distribution

$$m(x) = m_0\left(1 + \kappa x^2\right), \tag{4.4}$$

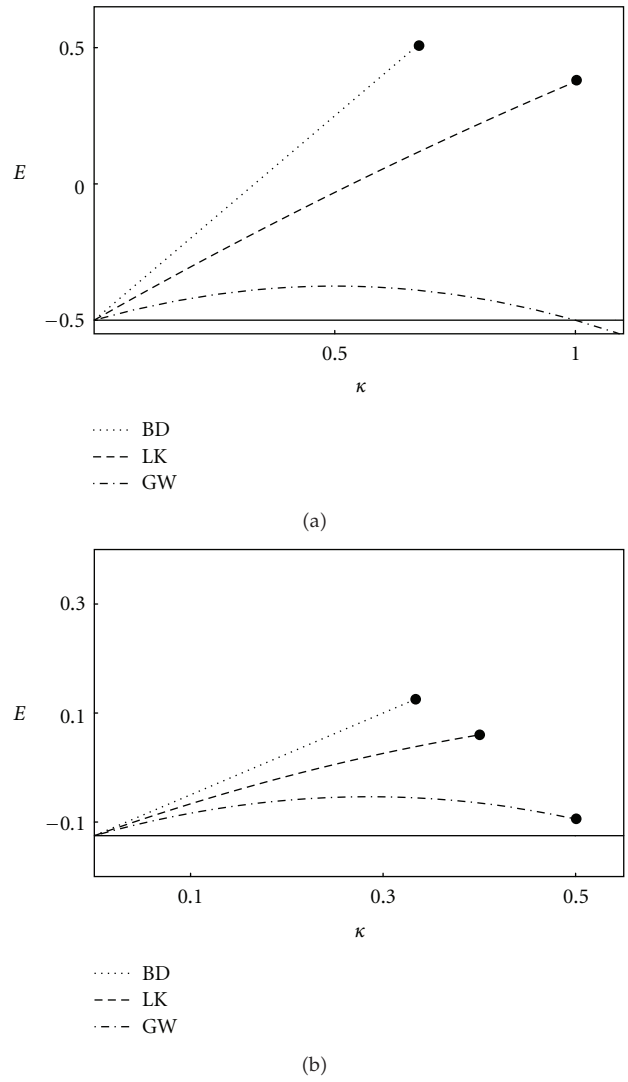

Figure 1: Energy for the states (a) ($n = 1, l = 0$) and (b) ($n = 2, l = 0$), in the Coulomb potential and the mass distribution (4.1), calculated with $\hbar = m_0 = Ze^2 = 1$. The solid line is the constant-mass result; the dotted, dashed, and dash-dotted curves are the PDM results obtained with Hamiltonians (3.8), (3.9), and (3.10), respectively.

which is found to be useful for studying quantum wells [3]. Applying Theorem 3.1 to this PDM profile, we get the inequality $E^{(\mathrm{BD})} \leq E^{(0)}$ that justifies the shift of electron and hole binding energies to lower values which was observed in [3] when the spatial dependence of mass was included. On the other hand, Theorem 3.2 does not apply since the quantity $\nabla^2(1/m(x)) = \kappa(6\kappa x^2 - 2)/m_0(1 + \kappa x^2)^3$ has an indefinite sign.

It is worth examining how this sign indefiniteness affects the energy spectrum. To that end, we choose the harmonic-oscillator potential, $V(x) = (1/2)m_0\omega^2 x^2$, for which the accurate numerical solution of the PDM Schrödinger equation with the mass distribution (4.4) is available [15]. In Figure 2, we plot the corresponding energy of the ground and the fifth

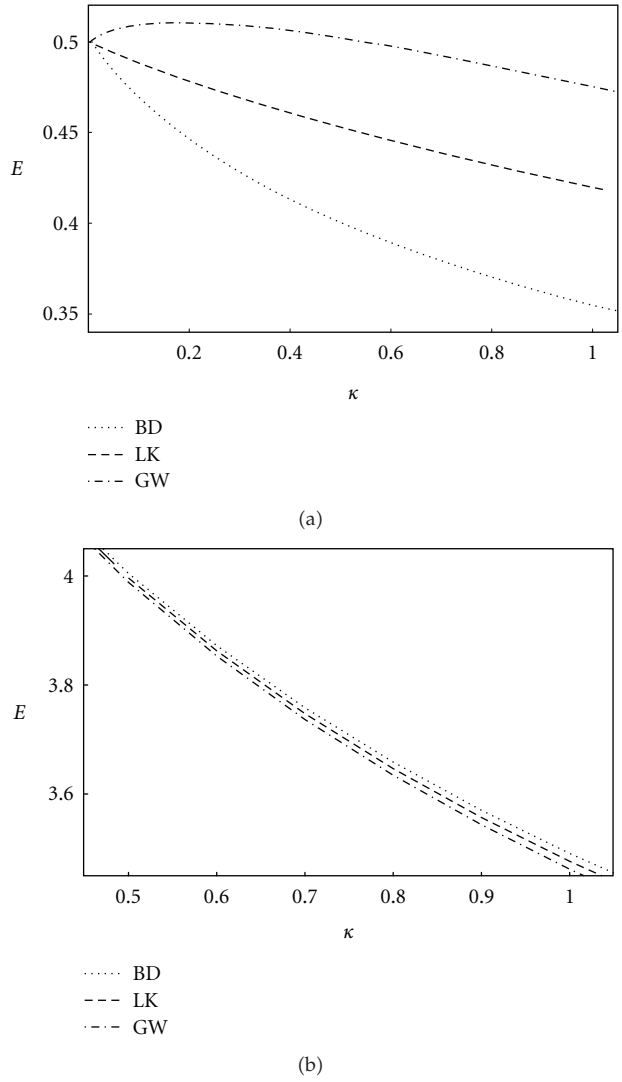

Figure 2: Energy for the states (a) $n = 0$ and (b) $n = 5$, in the harmonic-oscillator potential and the mass distribution (4.4), calculated with $\hbar = m_0 = \omega = 1$. The dotted, dashed, and dash-dotted curves are the PDM results obtained with Hamiltonians (3.8), (3.9), and (3.10), respectively.

excited states, as a function of κ, for the three PDM Hamiltonians with different ambiguity parameters. The energies have been calculated with $\hbar = m_0 = \omega = 1$, by using the shooting method, and are in agreement with those computed in [15] where the results obtained with the same m_0 and ω, and $\kappa = 0.1$ are reported.

From Figure 2, it is evident that for the excited state the discrepancy among the energies evaluated using the different PDM Hamiltonians is less profound. However, we call attention to a serious difference between the ground and excited states. As seen in Figure 2, the ground-state energies are ordered as $E^{(\mathrm{BD})} < E^{(\mathrm{LK})} < E^{(\mathrm{GW})}$ whereas the energies of the fifth excited state (and of the states with $n > 5$) are in inverse order. This inversion can be easily understood in conjunction with Theorem 3.2. It is known that the wave functions of highly ex-

cited states are spread to larger distances. Consequently, with increasing n, the mean value of x^2 grows and eventually reaches the point where the sign of $\nabla^2(1/m(x))$ in Theorem 3.2 reverses, thus inverting the order of energies.

5. Summary

In this paper, we have established the comparison theorems for the PDM Schrödinger equation. Our first theorem states that the corresponding eigenvalues of a constant-mass Hamiltonian and of a BenDaniel-Duke PDM Hamiltonian with the same potential are ordered if the constant and position-dependent masses are ordered everywhere. The second theorem concerns PDM Hamiltonians with the different sets of ambiguity parameters: the BenDaniel-Duke, Li-Kuhn, and Gora-Williams Hamiltonians. It is proved that their corresponding eigenvalues are ordered if the Laplacian of the inverse mass distribution $1/m(\mathbf{x})$ has a definite sign.

We have applied these theorems to the PDM Coulomb and harmonic-oscillator problems and have been led to the following conclusions. First, the eigenvalues of PDM Hamiltonians other than the BenDaniel-Duke one do not have to be in the strict order with respect to the eigenvalues of the constant-mass Hamiltonian. For instance, from both Figures 1 and 2, it is seen that the order of the Gora-Williams and constant-mass ground-state energies do vary, depending on the value of the deforming parameter κ. Second, if the quantity $\nabla^2(1/m(\mathbf{x}))$ has no definite sign and thus Theorem 3.2 does not apply, then the order of the energies calculated using different PDM Hamiltonians may alternate, as seen by comparing parts (a) and (b) of Figure 2. We therefore think that for establishing further comparison rules within the PDM framework one should restrict the potential profile to, for example, a spherically symmetric case, the way the generalized comparison theorems for the ordinary Schrödinger equation have been obtained [27].

The comparison rules we have found out can be employed for analyzing the energy spectra in semiconductor nanodevices; an example of application to the quantum well system was sketched in the previous section. In this connection, it is worthwhile to extend the present approach to periodic heterostructures, which allow the direct fit of PDM binding energies to experiment [25]. Then, we will have to abandon the requirement of vanishing of the wave function at infinity which the proof of our theorems relies on. What comparison rules might be formulated in that case is an interesting open question.

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