Position-dependent mass momentum operator and minimal coupling: point canonical transformation and isospectrality

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Abstract: The classical and quantum mechanical correspondence for constant mass settings is used, along with some nonlocal point transformation, to find the position-dependent mass (PDM) classical and quantum Hamiltonians. The comparison between the resulting quantum PDM-Hamiltonian and the von Roos PDM-Hamiltonian implied that the ordering ambiguity parameters of von Roos are strictly determined. Eliminating, in effect, the ordering ambiguity associated with the von Roos PDM-Hamiltonian. This, consequently, played a vital role in the construction/identification of the PDM-momentum operator. The same recipe is followed to identify the form of the minimal coupling of electromagnetic interactions for the classical and quantum PDM-Hamiltonians. It turned out that the minimal coupling of the electromagnetic interactions inherits the usual forms but with PDM pseudo-momentum (operator) rather than the usual momentum (operator). That is, \( \pi_j(\vec{x}) \to \pi_j(\vec{x}) - e A_j(\vec{x}) \) for the classical PDM-Hamiltonian, and \( \hat{\pi}_j(\vec{x}) \to \hat{\pi}_j(\vec{x}) - e A_j(\vec{x}) \) for the quantum PDM-Hamiltonian operator, where \( \pi_j(\vec{x}) \) is the \( j \)th component of the classical PDM pseudo-momentum and \( \hat{\pi}_j(\vec{x}) \) is the \( j \)th component of the quantum PDM pseudo-momentum operator. Two commonly used vector potential \( A_j(\vec{x}) \) are considered as Illustrative examples.

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I. INTRODUCTION

When the information on the material properties is encoded in the mass of a quantum particles, the concept of quantum particles endowed with position-dependent mass (PDM) becomes unavoidable. To deal with such quantum mechanical problems, von Roos [1] has suggested a PDM Hamiltonian of the form

\[
\hat{H} = -\frac{1}{4} \left[ M(\vec{x})^\alpha \partial_{x_j} M(\vec{x})^\beta \partial_{x_j} M(\vec{x})^\gamma + M(\vec{x})^\gamma \partial_{x_j} M(\vec{x})^\beta \partial_{x_j} M(\vec{x})^\alpha \right] + V(\vec{x}).
\]

(1)

Where \( M(\vec{x}) = m_0 m(\vec{x}) \), \( m_0 \) is the rest mass, \( m(\vec{x}) \) is a position-dependent dimensionless scalar multiplier that forms the position-dependent mass \( M(\vec{x}) \), \( \vec{x} = (x_1, x_2, x_3) \), \( \partial_{x_j} = \partial/\partial x_j \), \( j = 1, 2, 3 \), \( V(\vec{x}) \) is the potential force field, and the summation runs over repeated indices, unless otherwise mentioned. This Hamiltonian has been a subject of interest over the last few decades not only as a mathematically challenging Hamiltonian but also as a feasibly applicable one in many field of physics. Obviously, a parametric ordering ambiguity (i.e., in \( \alpha, \beta, \) and \( \gamma \)) arises in the formation of such Hamiltonian as a consequence of the non-unique representation of the kinetic energy term. It is known that, the ordering ambiguity parameters \( \alpha, \beta, \) and \( \gamma \) only satisfy the von Roos constraint \( \alpha + \beta + \gamma = -1 \). A constraint that is, in fact, manifested by the requirement that the von Roos Hamiltonian should collapse into the constant mass Hamiltonian settings as \( m(\vec{x}) = 1 \).

Many attempts were made to come out with a physically acceptable parametric ordering settings [2-12]. The only physically acceptable condition (along with the von Roos constraint) on the ambiguity parametric setting is that \( \alpha = \gamma \) to ensure the continuity condition at the abrupt heterojunction between two crystals (c.f., e.g., Ref. [13]). The rest were either based on circumstantial ordering settings that fit into exact solvability requirement, or those of mathematical and classical mechanical challenging nature [14-48], or even those that are based on an intelligent guess of the factorization structure of the kinetic energy operator (c.f., e.g., [49, 50] and related references cited therein). To the best of our knowledge, however, no attempts were ever made to construct and identify the PDM-momentum operator. We do this as part of the current methodical proposal. Nevertheless, it should be noted that Hamiltonian

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(1) would, in a straightforward manner, imply a time-independent PDM Schrödinger equation (in \( h = 2m_o = c = 1 \) units) of the form

\[
\begin{align*}
&\left\{ -\frac{1}{m(\vec{x})}\partial_{x_j}^2 + \frac{\partial_x m(\vec{x})}{m(\vec{x})^2} \partial_{x_j} \right. - [\alpha (\alpha + \beta + 1) + \beta + 1] \left( \frac{\partial_x m(\vec{x})^2}{m(\vec{x})^4} \right) \\
&\left. + \frac{1}{2} (1 + \beta) \left( \frac{\partial^2_x m(\vec{x})}{m(\vec{x})^2} \right) \right) + V(\vec{x}) \phi(\vec{x}) = E \phi(\vec{x}). \tag{2}
\end{align*}
\]

This equation is to play a critical role in the determination of the ambiguity parameters setting and consequently in the construction of the PDM-momentum operator as well as in the identification of the minimal coupling of electromagnetic interactions. The organization of the current methodical proposal is in the respective order, therefore.

In section II, we start with the Lagrangian of a classical particle of mass \( m_o \) moving a scalar potential field \( V(\vec{q}) \) in the generalized coordinates \( \vec{q} = (q_1, q_2, q_3) \) to build up the classical and consequently the quantum mechanical Hamiltonians. Based on our very recent work on the so called nonlocal point transformation [33], we detail out the mapping(s)/connection(s) between the quantum mechanical PDM-Schrödinger equation (2) and the apparently standard textbook Schrödinger equation for constant mass \( m_o \) in the generalized coordinates (obtained as a quantum mechanical correspondence of the classical Hamiltonian). Once the mapping is made clear, the ordering ambiguity in (2) disappears and the parametric setting become strictly determined. However, a question of delicate nature arises in the process as to "what is the form of the position-dependent mass momentum operator, if there is any at all?". In section III, we find that the answer to this question in the very fundamentals of "Quantum Mechanics" of S. Gasiorowicz [61] (equation (17) and (18) below). In so doing, we first find the so called PDM pseudo-momentum operator \( \hat{\pi}_j(\vec{x}) \) (obtained early on using a factorization method by Mustafa and Mazarimousavi in [43]) and connect it with the PDM-momentum operator through \( \hat{P}_j(\vec{x}) = \sqrt{m(\vec{x})} \hat{\pi}_j(\vec{x}) \). Surprisingly, it turns out that the construction of the PDM pseudo-momentum operator (hence, PDM-momentum operator) has nothing to do with the ambiguity parameters but it only depends on the transformation of the wave function form the generalized coordinate \( \vec{q} = (q_1, q_2, q_3) \) into the rectangular coordinates \( \vec{x} = (x_1, x_2, x_3) \) (i.e., \( \psi(\vec{q}) \rightarrow m(\vec{x})^{-\alpha} \phi(\vec{x}) \), equation (14) below.

Next, having the PDM-momentum (operator) identified in both the classical and quantum mechanical forms, we dwell on the nature of the minimal coupling of electromagnetic interactions for PDM-settings in section IV. Therein, we find out that the simplest way of coupling the electromagnetic interaction is to take the Hamilton’s PDM pseudo-momentum \( \pi_j(\vec{x}) \) as the sum of the PDM pseudo-kinetic momentum \( m_o \hat{q}_j = m_o \left( \sqrt{m(\vec{x})} \dot{x}_j \right) \) and \( e A_j(\vec{x}) \) (i.e., \( \pi_j(\vec{x}) = m_o \left( \sqrt{m(\vec{x})} \dot{x}_j \right) + e A_j(\vec{x}) \)). Hence, the minimal coupling of the electromagnetic interactions turns out to be \( \pi_j(\vec{x}) \rightarrow \pi_j(\vec{x}) - e A_j(\vec{x}) \) and \( E = H \rightarrow E - e \varphi(\vec{x}) \) for the Classical PDM-Hamiltonian and, likewise, \( \hat{\pi}_j(\vec{x}) \rightarrow \hat{\pi}_j(\vec{x}) - e A_j(\vec{x}) \) and \( E \rightarrow E - e \varphi(\vec{x}) \) for the Quantum PDM-Hamiltonian, where \( \hat{\pi}_j(\vec{x}) \) is the \( j^{th} \) component of the PDM pseudo-momentum operator, \( E \) is the eigenenergy and \( e \varphi(\vec{x}) \) is the scalar part of the electromagnetic four vector potential \( A_\mu = (\vec{A}(\vec{x}), \varphi(\vec{x})) \).

In section V we give some illustrative examples considering two commonly used vector potentials. We conclude in section VI.

II. POINT TRANSFORMATION AND CLASSICAL-QUANTUM CORRESPONDENCE

Consider the motion of a classical particle of a constant rest mass \( m_o \) moving in a potential field \( V(\vec{q}) \), where \( \vec{q} = (q_1, q_2, q_3) = q_1 \tilde{q}_1 + q_2 \tilde{q}_2 + q_3 \tilde{q}_3 \) are the generalized coordinates. The corresponding Lagrangian for such a system is given by

\[
L(q_j, \dot{q}_j; \tau) = \frac{1}{2} m_o \dot{q}_j^2 - V(\vec{q}); \quad \dot{q}_j = \frac{dq_j}{d\tau} \quad j = 1, 2, 3. \tag{3}
\]

Where \( \tau \) is a re-scaled time [39] and \( L(q_j, \dot{q}_j; \tau) = L(q_1, q_2, q_3, \dot{q}_1, \dot{q}_2, \dot{q}_3; \tau) \) is to be used for the economy of notations. Under such settings, the classical Hamiltonian reads

\[
H(q_j, P_j; \tau) = \dot{q}_j P_j - L(q_j, \dot{q}_j; \tau) = \frac{1}{2} m_o \dot{q}_j^2 + V(\vec{q}), \tag{4}
\]

and represents a constant of motion where \( dH(q_j, P_j; \tau) / d\tau = 0 \) (c.f., e.g., Mustafa [39]). Here, the \( j^{th} \) component of the generalized (canonical) momentum (associated with the generalized coordinate \( q_j \))

\[
P_j = \frac{\partial}{\partial \dot{q}_j} L(q_j, \dot{q}_j; \tau) \implies P_j = m_o \dot{q}_j, \tag{5}
\]
is used. However, the Hamiltonian is often realized to be a function of position \( q_j \) and canonical momentum \( P_j \) (and not a function of position \( q_j \) and velocity \( \dot{q}_j \)). It is more appropriate, therefore, to re-cast the classical Hamiltonian (4) as

\[
H (q_i, P_j; \tau) = \frac{1}{2m_\omega} P_j^2 + V(q). 
\]  
(6)

Hence, the corresponding quantum mechanical Hamiltonian is obtained by the identification of the \( j \)th canonical momentum \( P_j \) with the operator \( \hat{P}_j = -i \partial / \partial q_j = -i \partial / \partial q_j \), that satisfies the canonical commutation relations \( [q_i, P_j] = -i \delta_{ij} \) and consequently yields (with \( \hbar = 2m_\omega = c = 1 \)) to

\[
\hat{H} (q_i, P_j; \tau) = -\partial_{q_j}^2 + V(q). 
\]  
(7)

Then, the corresponding time-independent Schrödinger equation reads

\[
\left\{ -\partial_{q_j}^2 + V(q) \right\} \psi (q) = \Lambda \psi (q) 
\]  
(8)

At this very point, we would like to figure out the mapping(s)/connection(s) between the quantum mechanical PDM-Schrödinger equation (2) and the apparently standard textbook Schrödinger equation for constant mass in (8) (equation (8) is obtained as a quantum mechanical correspondence of the classical Hamiltonian (6)). To do that, we invest in our experience on the nonlocal point transformation very recently suggested by Mustafa [39] and define

\[
dq_j = \delta_{ij} \sqrt{g(\bar{x})} \, dx_j = \sqrt{g(\bar{x})} \, dx_j \implies \frac{dq_j}{dx_j} = \delta_{ij} \sqrt{g(\bar{x})} \implies q_j = \int \sqrt{g(\bar{x})} \, dx_j, \quad \tau = \int f(\bar{x}) \, dt. 
\]  
(9)

No summation over repeated index holds in (9). Therefore, this type of transformation necessarily means that the differential change in \( q_j \) is defined through the matrix

\[
\begin{bmatrix}
\frac{dq_1}{dx_1} \\
\frac{dq_2}{dx_2} \\
\frac{dq_3}{dx_3}
\end{bmatrix} = \begin{bmatrix}
\frac{\partial q_1}{\partial x_1} & 0 & 0 \\
0 & \frac{\partial q_2}{\partial x_2} & 0 \\
0 & 0 & \frac{\partial q_3}{\partial x_3}
\end{bmatrix} \begin{bmatrix}
dx_1 \\
dx_2 \\
dx_3
\end{bmatrix} = \sqrt{g(\bar{x})} \begin{bmatrix}
dx_1 \\
dx_2 \\
dx_3
\end{bmatrix} \implies \hat{q}_j = \sqrt{g(\bar{x})} \hat{x}_j; \quad \hat{x}_j = \frac{dx_j}{dt}. 
\]  
(10)

Consequently, the unit vectors in the direction of \( q_j \) are obtained as

\[
\hat{q}_j = \sqrt{g(\bar{x})} \left[ \left( \frac{\partial x_1}{\partial q_j} \right) \hat{x}_1 + \left( \frac{\partial x_2}{\partial q_j} \right) \hat{x}_2 + \left( \frac{\partial x_3}{\partial q_j} \right) \hat{x}_3 \right] \implies \hat{q}_i = \hat{x}_i. 
\]  
(11)

Moreover, one should notice that such a point transformation recipe, along with the condition \( g(\bar{x}) = m(\bar{x}) f(\bar{x})^2 \), would keep the related Euler-Lagrange equations invariant (for more detailed analysis on this issue one may refer to Mustafa [39]). Therefore, the related time-independent Schrödinger equation would, with the substitutions of

\[
\psi (q) = g(\bar{x})^v \phi (\bar{x}), 
\]  
(12)

yield

\[
\left\{ -\frac{1}{g(\bar{x})} \partial_{\bar{x}_j}^2 - \left( 2v - \frac{1}{2} \right) \left( \frac{\partial x_i g(\bar{x})}{g(\bar{x})^2} \right) \partial_{\bar{x}_j} - v \left( v - \frac{3}{2} \right) \left( \frac{[\partial x_i g(\bar{x})]^2}{g(\bar{x})^3} \right) \right. \\
- v \left( \frac{\partial_{\bar{x}_j}^2 g(\bar{x})}{g(\bar{x})^2} \right) + V(q) \left\} \phi (\bar{x}) = \Lambda \phi (\bar{x}). 
\]  
(13)

Nevertheless, we shall be interested in quantum mechanical systems in (8) that are exactly solvable, conditionally exactly solvable, or quasi-exactly solvable to reflect on the solvability of a given PDM system as in (13). Therefore, the eigenvalues \( \Lambda \) of (13) should be not only position independent but also isospectral to \( E \) of (2), i.e., \( E = \Lambda \). Under such settings, one immediately concludes that \( f(\bar{x}) = 1 \implies \tau = t \) and \( g(\bar{x}) = m(\bar{x}) \) to keep the total energy position-independent and ensures isospectrality between (2) and (8). Now, we compare the second term of (2) with second term of (13) to imply that

\[
2v - \frac{1}{2} = -1 \implies v = -\frac{1}{4} \implies \psi (q) = m(\bar{x})^{-1/4} \phi (\bar{x}). 
\]  
(14)
Hence (13) reduces to
\[
\begin{align*}
\left\{- \frac{1}{m(\vec{x})} \partial^2_{x}\right\} + \left[ \frac{\partial_{x}m(\vec{x})}{m(\vec{x})^2} \right] \partial_{x} - \frac{7}{16} \left( \frac{\partial_{x}m(\vec{x})}{m(\vec{x})^3} \right)^2 + \frac{1}{4} \left[ \frac{\partial^2_{x}m(\vec{x})}{m(\vec{x})^2} \right] + V(q(\vec{x})) \right\} \phi(\vec{x}) = E \phi(\vec{x}).
\end{align*}
\]

Consequently, moreover, one obtains the identities
\[
\alpha (\alpha + \beta + 1) + \beta + 1 = \frac{7}{16}, \quad \frac{1}{2} (1 + \beta) = \frac{1}{4}.
\]

Equations (8) and (15) are isospectral (i.e., they share the same energy spectra). Yet, the comparison clearly suggests that the ordering ambiguity parameters are strictly determined in (16) (along with the von Roos constraint $\alpha + \beta + \gamma = -1$) as $\beta = -1/2$, and $\alpha = -1/4 = \gamma$. The result that $\alpha = \gamma = -1/4$ satisfy the continuity condition at the abrupt heterojunction between two crystals (c.f., e.g., Ref. [13]). In the literature, this ordering is known as MM-ordering of Mustafa and Mazharimousavi [49, 50]. Hereby, we may safely conclude that the PDM quantum mechanical correspondence of the PDM classical mechanical settings leads to MM-ordering and removes the ordering ambiguity in the von Roos PDM-Hamiltonian (1). We adopt MM-ordering parameters and proceed with the point transformation settings used above.

### III. CONSTRUCTION OF THE PDM-MOMENTUM OPERATOR

Having the correlation between the Schrödinger equation (in the generalized coordinates) and the PDM-Schrödinger equation (in the rectangular coordinates) been identified, through (8)-(15), we now need to address a question of delicate nature as to "what is the form of the position-dependent mass momentum operator, if there is any at all?". The answer to this question very well lies in the very fundamentals of "Quantum mechanics" by S. Gasiorowicz [51]. Therein, the one-dimensional quantum mechanical momentum operator $\hat{p}_x = -i\partial/\partial x$ is determined through

\[
\langle p_x \rangle = m_{\omega} \frac{d}{dx} \langle x \rangle = \int_{-\infty}^{\infty} dx \Psi^* (x, t) \left(-i \frac{\partial}{\partial x}\right) \Psi (x, t) \Rightarrow \hat{p}_x = -i\partial/\partial x.
\]

This would suggest that the one-dimensional quantum momentum operator in the generalized coordinate $q$ for the one-dimensional quantum mechanical system is also obtainable through the same recipe as

\[
\langle P_q \rangle = m_{\omega} \frac{d}{dq} \langle q \rangle = \int_{-\infty}^{\infty} dq \Psi^* (q, t) \left(-i \frac{\partial}{\partial q}\right) \Psi (q, t) \Rightarrow \hat{P}_q = -i\partial/\partial q.
\]

Which is, in fact, what we have readily used above. Of course, the details of the intermediate steps are straightforward and hold true for both (17) and (18) and need not be recycled here. Next, if we use the corresponding one-dimensional point transformations

\[
dq = \sqrt{m(x)} dx, \quad \frac{\partial x}{\partial q} = \frac{1}{\sqrt{m(x)}},
\]

and $\Psi (q, \tau) = m(x)^{-1/4} \Phi (x, t)$ in (18), we immediately get

\[
\langle P_q \rangle = \int_{-\infty}^{\infty} dx \sqrt{m(x)} \left[ \frac{\Phi^* (x, t)}{m(x)^{1/4}} \right] \left( -i \sqrt{m(x)} \frac{\partial}{\partial x} \right) \left[ \frac{\Phi (x, t)}{m(x)^{1/4}} \right] = \int_{-\infty}^{\infty} dx \Phi^* (x, t) \left( \frac{\partial}{\sqrt{m(x)} \partial x} - \frac{1}{4} \left( \frac{\partial x m(x)}{m(x)} \right) \right) \Phi (x, t) \Rightarrow \hat{P}_q (x) = \frac{1}{\sqrt{m(x)}} \left[ \frac{\partial}{\partial x} - \frac{1}{4} \left( \frac{\partial x m(x)}{m(x)} \right) \right] \Phi (x, t)
\]

Hereby, one should notice that the construction of this PDM momentum-like operator (descending from the generalized coordinates settings into rectangular settings) has nothings to do with ambiguity parameters $\alpha, \beta$, and $\gamma$. It is only a manifestation of mapping the wave functions from one coordinate system to another through (19). This is not yet the PDM-momentum operator and shall be called PDM pseudo-momentum operator (with the identity $\pi_x (x)$), exactly.
the same as the one obtained by a factorization method by Mustafa and Mazharimousavi in [49]. The generalization of which is straightforward and takes the form

$$\hat{\pi}_j (\vec{x}) = -i \frac{1}{\sqrt{m(\vec{x})}} \left[ \frac{\partial}{\partial x_j} - \frac{1}{4} \left( \frac{\partial_{x_j} m(\vec{x})}{m(\vec{x})} \right) \right]$$

$$\iff \hat{\pi}(\vec{x})_{\text{op.}} = \frac{-i}{\sqrt{m(\vec{x})}} \left[ \vec{\nabla} - \frac{1}{4} \left( \vec{\nabla} m(\vec{x}) \right) \right],$$

(21)

where \(\hat{\pi}_j (\vec{x}) \rightarrow \hat{p}_j = -i \partial/\partial x_j\) for constant mass settings (i.e., the dimensionless scalar multiplier \(m(\vec{x}) = 1\)). In fact, equation (21) gives the differential form of the Hamilton’s canonical PDM pseudo-momentum operator \(\hat{\pi}(\vec{x})_{\text{op.}}\).

Under such settings, our PDM Schrödinger equation (15) inherits the usual simplistic form as

$$\{ \hat{\pi}_j^2 (\vec{x}) + V(\vec{x}) \} \phi(\vec{x}) = E \phi(\vec{x}).$$

(22)

Furthermore, one should be aware that for \(2m_o \neq 1\) the first term of equation (22) would result in \(\hat{\pi}_j^2 (\vec{x})/2m_o\) as the quantum PDM-kinetic energy operator (i.e., \(\hat{T} = \hat{\pi}_j^2 (\vec{x})/2m_o\)). Only under such transformation procedure’s settings the quantum Hamiltonian implies the classical one, the other way around holds true as well. That is,

$$\hat{H}_{\text{quantum}} = \frac{\hat{\pi}_j^2 (\vec{x})}{2m_o} + V(\vec{x}) \iff H_{\text{classical}} = \frac{1}{2} m_o m(\vec{x}) \dot{x}_j^2 + V(\vec{x}) = \frac{\pi_j^2 (\vec{x})}{2m_o} + V(\vec{x})$$

(23)

where \(\pi_j(\vec{x})\) is the \(j\)th-component of the classical PDM pseudo-momentum obtained through

$$\dot{q}_j (\vec{x}) = \sqrt{m(\vec{x})} \dot{x}_j \Rightarrow \frac{dq_j}{dt} = \hat{q}_j \hat{\pi}_j = \sqrt{m(\vec{x})} \dot{x}_j \Rightarrow \pi_j (\vec{x}) = m_o \sqrt{m(\vec{x})} \dot{x}_j,$$

(24)

and \(\hat{\pi}_j (\vec{x})\) is the corresponding \(j\)-th-component of the quantum PDM pseudo-momentum operator. At this very point, however, one recollects the classical PDM-Lagrangian \(L = m_o m(\vec{x}) \dot{x}_j^2/2 - V(\vec{x})\) to imply the classical PDM Hamiltonian \(H = m_o m(\vec{x}) \dot{x}_j^2/2 + V(\vec{x}) = P_j^2 / (2m_o m(\vec{x})) + V(\vec{x})\) where \(\dot{P}_j (\vec{x}) = \partial L / \partial \dot{x}_j = m_o m(\vec{x}) \dot{x}_j\) is the canonical PDM-momentum. This would, in effect, imply that \(P_j (\vec{x}) = \sqrt{m(\vec{x})} \pi_j (\vec{x})\) and consequently the PDM-momentum operator reads

$$\hat{P}_j (\vec{x}) = \sqrt{m(\vec{x})} \hat{\pi}_j (\vec{x}) = -i \left[ \frac{\partial}{\partial x_j} - \frac{1}{4} \left( \frac{\partial_{x_j} m(\vec{x})}{m(\vec{x})} \right) \right] \iff \hat{\pi}_j (\vec{x}) = \frac{\hat{P}_j (\vec{x})}{\sqrt{m(\vec{x})}},$$

where \(\hat{\pi}_j (\vec{x})\) is given in (21). This would necessarily mean that \(\hat{\pi}_j^2 (\vec{x})\) of (22) should be expressed as \(\left( \hat{P}_j (\vec{x}) / \sqrt{m(\vec{x})} \right)^2\) and not as \(\hat{P}_j^2 (\vec{x})/m(\vec{x})\). In classical mechanics both forms work but not in quantum mechanics. We are now in a position to dwell on electromagnetic interaction and minimal coupling for PDM settings using our PDM pseudo-momentum operator \(\hat{\pi}_j (\vec{x})\) for the sake of simplicity and convenience.

IV. CLASSICAL ELECTROMAGNETIC INTERACTION AND THE PDM-QUANTUM MECHANICAL CORRESPONDENCE

In this section, we adopt our procedure above and extend it to include electromagnetic interactions. This would, in effect, allow us to have an idea as to “how the minimal coupling for PDM settings is integrated into the PDM Schrödinger equation (22)? and what form would it take?”. Hereby, we begin with the motion of a classical particle of charge \(e\) and a constant rest mass \(m_o\) moving in an electromagnetic interaction represented by the 4-vector potential \(A_\mu = (\vec{A}, i \varphi)\) with the vector potential \(\vec{A}(\vec{q})\) and a scalar potential \(\varphi(\vec{q})\). The Lagrangian for such a system is given by

$$L(q_j, \dot{q}_j; t) = \frac{1}{2} m_o \dot{q}_j^2 + e \dot{q}_j A_j (\vec{q}) - |e \varphi(\vec{q}) + V(\vec{q})| ; \dot{q}_j = \frac{dq_j}{dt},$$

(25)

Where \(V(\vec{q})\) is any other potential energy than the electric and magnetic ones. Of course, this is a more general problem than the one discussed in section II and one may switch-off the electromagnetic interaction potentials (i.e., \(A_j (\vec{q}) = 0\) and \(\varphi(\vec{q}) = 0\) and, therefore, recover the same results discussed therein.
Under such Lagrangian (25) settings, the classical Hamiltonian reads

\[ H (q_j, P_j; t) = \dot{q}_j P_j - L (q_j, \dot{q}_j; t) = \frac{1}{2} m_o \dot{q}_j^2 + W (\dot{q}); \quad W (\dot{q}) = e \varphi (\dot{q}) + V (\dot{q}). \] (26)

Here, the \( j \)th component of the generalized (canonical) momentum (associated with the generalized coordinate \( q_j \)) is given by

\[ P_j = \frac{\partial}{\partial \dot{q}_j} L (q_j, \dot{q}_j; t) \implies P_j = m_o \dot{q}_j + e A_j (\dot{q}), \] (27)

and the classical Hamiltonian (26) takes the form

\[ H (q_j, P_j; t) = \frac{1}{2 m_o} (P_j - e A_j (\dot{q}))^2 + W (\dot{q}). \] (28)

Hence, the corresponding quantum mechanical Hamiltonian, with \( \hat{P}_j = -i \partial_{\dot{q}_j} \), consequently yields

\[ \hat{H} (q_j, P_j; t) = -\partial^2_{\dot{q}_j} + i e [\partial_{\dot{q}_j} A_j (\dot{q}) + 2 i e A_j (\dot{q}) \partial_{\dot{q}_j} + e^2 A_j (\dot{q})^2 + W (\dot{q})]. \] (29)

Now, we follow our methodical proposal in section II above and obtain the corresponding time-independent PDM-Schrödinger equation

\[
\begin{cases}
- \frac{1}{m (\vec{x})} \frac{\partial^2}{\partial x_j^2} + \frac{\partial_x m (\vec{x})}{m (\vec{x})^2} \partial_{x_j} - \frac{7}{16} \left( \frac{\partial_x m (\vec{x})}{m (\vec{x})} \right)^2 + \frac{1}{4} \left( \frac{\partial_x^2 m (\vec{x})}{m (\vec{x})^2} \right) - i e \frac{\partial_x A_j (\vec{x})}{\sqrt{m (\vec{x})}} \\
+ 2 i e \frac{A_j (\vec{x})}{\sqrt{m (\vec{x})}} \left( \partial_{x_j} - \frac{1}{4} \left( \frac{\partial_x m (\vec{x})}{m (\vec{x})} \right) \right) + e^2 A_j (\vec{x})^2 + W (\vec{x}) \end{cases}
\]

that reduces to

\[
\left\{ \left[ \frac{-i}{\sqrt{m (\vec{x})}} \left( \frac{\partial}{\partial x_j} - \frac{1}{4} \left( \frac{\partial_x m (\vec{x})}{m (\vec{x})} \right) \right) - e A_j (\vec{x}) \right]^2 + W (\vec{x}) \right\} \phi (\vec{x}) = E \phi (\vec{x}).
\] (30)

or in a more simplistic format

\[
\left\{ \left[ \hat{\pi}_j (\vec{x}) - e A_j (\vec{x}) \right]^2 + W (\vec{x}) \right\} \phi (\vec{x}) = E \phi (\vec{x}) \tag{31}.
\]

Classical mechanically, therefore, the simplest way of coupling the electromagnetic interaction is to take the Hamilton’s canonical pseudo-momentum \( \pi_j (\vec{x}) \) as the sum of the kinetic momentum \( m_o \dot{q}_j = m_o \left( \sqrt{m (\vec{x})} \dot{x}_j \right) \) and \( e A_j (\vec{x}) \) (i.e., \( \pi_j (\vec{x}) = m_o \left( \sqrt{m (\vec{x})} \dot{x}_j \right) + e A_j (\vec{x}) \)). Hence, for the classical Hamiltonian in (23) one may simply use the minimal coupling

\[ \pi_j (\vec{x}) = \frac{P_j (\vec{x})}{\sqrt{m (\vec{x})}} \implies \pi_j (\vec{x}) - e A_j (\vec{x}) \quad \text{and} \quad E = H_{\text{classical}} \implies E - e \varphi (\vec{x}). \tag{33} \]

to incorporate electromagnetic interactions. Consequently, in quantum mechanics, it is obvious that the electromagnetic interactions for PDM are integrated into the PDM-Schrödinger equation (22) through the the minimal coupling

\[ \hat{\pi}_j (\vec{x}) = \frac{\hat{P}_j (\vec{x})}{\sqrt{m (\vec{x})}} \implies \hat{\pi}_j (\vec{x}) - e A_j (\vec{x}) \quad \text{and} \quad E \implies E - e \varphi (\vec{x}). \tag{34} \]

Which, in fact, looks very much like the usual constant mass settings but now with the Classical PDM pseudo-momentum \( \pi_j (\vec{x}) \) of (24) and the Quantum PDM pseudo-momentum operator \( \hat{\pi}_j (\vec{x}) \) of (21) rather than the textbook momentum \( p_j = m_o \dot{x}_j \) and momentum operator \( \hat{p}_j = -i \partial / \partial x_j \), respectively. This result renders the procedure followed by Dutra and Oliveira [10] inappropriate, for they have started with their equation (37), assuming that \( \hat{p}_j = -i \partial / \partial x_j \) and \( \hat{p}_j \rightarrow \hat{p}_j - e A_j (\vec{x}) \) (this recipe is correct only for constant mass settings). However, this readily lies far beyond our methodical proposal and shall be discussed elsewhere.
Nevertheless, one should notice that a proper reverse engineering of (32), with \( \phi(\vec{x}) = m (\vec{x})^{1/4} \psi(\vec{q}) \), would immediately yield
\[
\left\{ \left[ \dot{\vec{P}} - eA_j(\vec{q}) \right]^2 + W(\vec{q}) \right\} \psi(\vec{q}) = E\psi(\vec{q}) ; \quad \dot{\vec{P}} = -i\partial_\vec{q}
\] (35)

Which clearly introduces a paramagnetic contribution as \( 2ieA_j(\vec{q}) \partial_\vec{q} \), and a diamagnetic one as \( e^2A_j(\vec{q})^2 \) along with an electric field contribution as \( e \phi(\vec{q}) \) in the generalized coordinates. Obviously, equation (35) represents a textbook example which is known to be exactly or conditionally exactly solvable model for some \( W(\vec{q}) \) forms. The solutions of which can be mapped into the PDM Schrödinger equation (32). This is to be clarified in the forthcoming illustrative examples.

V. ILLUSTRATIVE EXAMPLES

In this section, we shall consider two vector potentials that satisfy the Coulomb gauge \( \partial_\vec{q}_iA_j(\vec{q}) = 0 \) and are often used in the literature as illustrative examples. They are,
\[
\vec{A}(\vec{q}) = B_0(-q_x,0,0) = -B_0 q_x \hat{q}_i
\] (36)

and
\[
\vec{A}(\vec{q}) = \frac{B_0}{2}(-q_x,q_y,q_z) = \frac{B_0}{2}(-q_x \hat{q}_i + q_x \hat{q}_i)
\] (37)

where \( \hat{q}_i \) is the unit vector for the generalized coordinate \( q_i \). Consequently, they result a constant magnetic
\[
\vec{B}(\vec{q}) = \nabla_\vec{q} \times \vec{A}(\vec{q}) = \left\{ \begin{array}{ll} B_0 \hat{q}_3 \text{ for } \vec{A}(\vec{q}) = B_0(-q_x,0,0) \\ \frac{B_0}{2} \hat{q}_3 \text{ for } \vec{A}(\vec{q}) = \frac{B_0}{2}(-q_x,q_y,q_z) \end{array} \right. : \nabla_\vec{q} = \hat{q}_i \partial_{q_i} + \hat{q}_j \partial_{q_j} + \hat{q}_k \partial_{q_k}
\] (38)

We start with Schrödinger equation (35) for different interaction potentials (be it the vector potentials \( \vec{q} \) and/or scalar potentials \( [e \phi(\vec{q}) + V(\vec{q})] \)) to reflect on the corresponding PDM settings in (32).

In so doing, we keep in mind our coordinates’ settings from (9) to (16) and choose, for both vector potentials above, to work with \( m(\vec{x}) = m(r) \); \( r = \sqrt{x^2 + y^2 + z^2} \), and a simple mapping where
\[
\partial_\vec{q}_i = \sqrt{m(\vec{x})} \partial_{x_j} = S(r) + \frac{x^2}{r} S'(r) , \text{ (no summation)}; \quad S'(r) = \frac{d}{dr} S(r).
\] (39)

Also by (9), with \( g(\vec{x}) = m(\vec{x}) \), we have
\[
\partial_\vec{q}_i = \sqrt{m(\vec{x})} = \sqrt{m(r)}; \text{ (no summation)} \Rightarrow 3\sqrt{m(r)} = 3S(r) + \frac{(x^2 + y^2 + z^2)}{r} S'(r),
\] (40)

to obtain
\[
\sqrt{m(r)} = S(r) + \frac{r}{N} S'(r) \iff S(r) = \frac{N}{r^3} \int r^2 \sqrt{m(r)} dr; \quad N = 3,
\] (41)

where \( S(r) \) is yet another dimensionless scalar multiplier like \( m(r) \). Although \( N = 3 \) for the current methodical proposal, we choose to cast the above equation in terms of \( N \) to identify the number of degrees of freedom involved in the problem at hand. Moreover, for a given \( m(r) \) one may find \( S(r) \) using (41), the other way around works as well. Therefore, \( m(r) \) and \( S(r) \) may very well be considered as generating functions of each other. That is, one may start with \( m(r) \) to find \( S(r) \), for example,
\[
m(r) = \frac{1}{1 + \lambda^2 r^2} \iff S(r) = \frac{2}{3} \left[ \frac{\sqrt{1 + \lambda^2 r^2}}{\lambda^2 r^2} - \frac{1}{\lambda^3 r^3} \ln \left( \lambda r + \sqrt{1 + \lambda^2 r^2} \right) \right] ; \quad \lambda > 0,
\] (42)
\[
m(r) = a^2 r^{2n} \iff S(r) = \frac{3}{n + 3} a r^n ; \quad a > 0, \quad n \neq -3,
\] (43)
\[
m(r) = a^2 r^{2n} \iff S(r) = \frac{3a}{r^3} \ln r ; \quad n = -3,
\] (44)
or one starts with $S(r)$ to find $m(r)$

\[
S(r) = br^n \iff m(r) = \frac{(3 + n)^2}{9}b^{2r+2n}; b > 0, n \neq -3,
\]

\[
S(r) = Br^n \ln r \iff m(r) = \frac{1}{9}B^2r^{2n}[(3 + n)\ln r + 1]^2,
\]

and so on so forth. In what follows, we clarify our methodical proposal.

\section{A. Charged particle in a vector potential $\vec{A}(\vec{q}) = B_o(-q_z, 0, 0)$ and $W(\vec{q}) = 0$}

Consider a charged particle in a vector potential $\vec{A}(\vec{q}) = B_o(-q_z, 0, 0)$ that results a constant magnetic field $\vec{B}(\vec{q}) = \vec{\nabla} \times \vec{A}(\vec{q}) \implies \vec{B}(\vec{q}) = B_o \hat{q}_3 = B_o \hat{x}_3$, equation (35) implies that

\[
\left\{ \left[ \hat{P}_1 + eB_0q_z \right]^2 + \hat{P}_2^2 + \hat{P}_3^2 \right\} \psi(\vec{q}) = E\psi(\vec{q}) \; ; \; \hat{P}_j = -i\partial_{q_j}.
\]

This would, in effect, suggest that the Hamiltonian $H(q, P) = \left[ \hat{P}_1 + eB_0q_z \right]^2 + \hat{P}_2^2 + \hat{P}_3^2$ does not explicitly depend on $q_1$ and $q_3$, and the commutation relations

\[
[q_j, \hat{P}_j] = i\delta_{ij}, \quad [\hat{P}_1, \hat{P}_2] = 0, \quad [\hat{P}_1, H(q, P)] = 0, \quad [\hat{P}_2, H(q, P)] = 0
\]

are satisfied. Hence, $\hat{P}_1$ and $\hat{P}_2$ are no longer operators but rather constants of motion (i.e., they are conserved and can be replaced by eigenvalues/numbers, therefore). Consequently, $\hat{P}_1 \rightarrow k_1, \hat{P}_3 \rightarrow k_3$ and the corresponding eigenfunction can very well be identified as

\[
\psi(\vec{q}) = \psi(q_1, q_2, q_3) = \exp[i(k_1q_1 + k_3q_3)] Q(q_2).
\]

Which, in turn, when substituted in (47) yields

\[
\left\{ -\frac{d^2}{dq_2^2} + c^2B_o^2 \left[ q_2 + \frac{k_1}{cB_o} \right]^2 + k_3^2 \right\} Q(q_2) = EQ(q_2).
\]

Obviously, this equation represents a standard textbook shifted-harmonic oscillator and can be rewritten as

\[
\left\{ -\frac{d^2}{dq_2^2} + \frac{1}{4} \omega^2 \eta^2 \right\} Q(\eta) = \{ E - k_3^2 \} Q(\eta) \; ; \; \eta = q_2 + k_1/cB_o, \omega = 2 |c| B_o,
\]

to obtain the energy eigenvalues

\[
E_n - k_3^2 = \left( n + \frac{1}{2} \right) \omega \implies E_n = k_3^2 + (2n + 1) |c| B_o; \quad n = 0, 1, 2, \ldots
\]

and eigen functions

\[
Q_n(\eta) \sim \exp\left[ -\frac{|c| B_o}{2} \eta^2 \right] H_n\left( \sqrt{|c| B_o} \eta \right)
\]

where $H_n\left( \sqrt{|c| B_o} \eta \right)$ are the Hermite polynomials.

\section{B. Charged particle in a vector potential $\vec{A}(\vec{q}) = B_o(-q_z, q_1, 0)$ and $W(\vec{q}) = 0$}

A charged particle moving under the influence of the vector potential $\vec{A}(\vec{q}) = B_o(-q_z, q_1, 0)/2 \implies \vec{B}(\vec{q}) = B_o \hat{q}_3/2 = B_o \hat{x}_3/2$ would be described by Schrödinger equation (35) as

\[
\left\{ \left[ \hat{P}_1 + \frac{eB_0}{2}q_z \right]^2 + \left[ \hat{P}_2 - \frac{eB_0}{2}q_1 \right]^2 + \hat{P}_3^2 \right\} \psi(\vec{q}) = E\psi(\vec{q}).
\]
The solution of which can be expressed as

\[ \psi (\bar{q}) = \exp \left[ i \left( k_0 q_1 + k_0 q_3 - \frac{eB_0}{2} q_2 \right) \right] Y (q_2) \]  

(55)

to result, again, a shifted harmonic oscillator like Schrödinger equation

\[ \left\{ - \frac{d^2}{dq_2^2} + e^2 B_0^2 \left[ q_2 - \frac{k_1}{eB_0} \right]^2 + k_3^2 \right\} Y_n (q_2) = E_n Y_n (q_2), \]  

(56)

Which admits exact energy eigenvalues and eigenfunctions, respectively, as

\[ E_n = k_3^2 + (2n + 1) |e| B_0, \]  

(57)

\[ Y_n (\zeta) \sim \exp \left[ \frac{-|e| B_0}{2} \zeta^2 \right] H_n \left( \sqrt{|e| B_0} \zeta \right); \quad \zeta = q_2 - \frac{k_1}{eB_0} \quad n = 0, 1, 2, \ldots \]  

(58)

For both vector potentials in the two subsections above, one may recollect our coordinates settings of (11) and (39), along with \( g (\tilde{x}) = m (\tilde{x}) \), to come out with

\[ \vec{A} (\tilde{q}(\tilde{x})) = S (\tilde{x}) \vec{A} (\tilde{x}) = \begin{cases} B_0 S (\tilde{x}) (-x_2, 0, 0) & \text{for } \vec{A} (\tilde{q}) = B_0 (-q_2, 0, 0) \\ \frac{B_0}{2} S (\tilde{x}) (-x_2, x_1, 0) & \text{for } \vec{A} (\tilde{q}) = B_0 (-q_2, q_1, 0) \end{cases}, \]  

(59)

where \( q_j = S (\tilde{x}) x_j, \tilde{x}_j \) (no summation), to build up the wave functions in the rectangular coordinates using \( \phi (\vec{x}) = m (\vec{x})^{1/4} \psi (\vec{q}) \) of (14) and choosing a PDM function as those exemplified in (42)-(46). Hereby, we notice that all PDM functions satisfying (41) share the same energy eigenvalues of either (52) or (57). Isospectrality is an obvious consequence of the current methodical proposal, of course.

**VI. CONCLUDING REMARKS**

In this paper, we have started with the PDM Lagrangian (3) for a classical particle of mass \( m_0 \) moving, in the generalized coordinates \( \tilde{q} = (q_1, q_2, q_3) \), under the influence of a scalar potential field \( V (\tilde{q}) \) and built up the corresponding classical Hamiltonian (6) as well as the quantum Hamiltonian operator (7). We have shown that the correlation between the associated time-independent Schrödinger equation (8), in the generalized coordinates, and the well known time-independent PDM Schrödinger equation (2) is an obvious consequence of a particular type of point transformation (9) (very recently used by Mustafa [39]) along with the transformation of the wave function (14). Using no other constraint than the von Roos one \( \alpha + \beta + \gamma = -1 \), it turned out that the ordering ambiguity in the von Roos Hamiltonian (1), vanishes as a result of comparison between the second terms of equation (2) and of (13). The ordering parameters are strictly determined as \( \beta = -1/2, \alpha = -1/4, \) and \( \gamma = -1/4 \) (documented in (14)-(16) and known in the literature as MM-ordering of Mustafa and Mazharimousavi [49, 50]). Hereby, in addition to the von Roos constraint, our parametric result that \( \alpha = \gamma \) satisfies and ensures the physically acceptable continuity condition at the abrupt heterojunction between two crystals (c.f., e.g., Ref. [13]). Yet, as a result of this comparison, we were able to use the correlation between the wave functions, i.e. \( \psi (\tilde{q}) = m (\tilde{x})^{-1/4} \phi (\tilde{x}) \), and construct the PDM pseudo-momentum operator in one dimension (see (17) and (20)) and generalize it to three dimensions in (21) (consequently, the PDM-momentum operator). In so doing, we have closely followed the very fundamentals of *Quantum mechanics* by S. Gasiorowicz [51]. To the best of our knowledge, the construction of the PDM-momentum operator

\[ \hat{P}_j (\tilde{x}) = \sqrt{m (\tilde{x})} \hat{x}_j (\tilde{x}) = -i \left[ \frac{\partial}{\partial x_j} - \frac{1}{4} \left( \frac{\partial x_j m (\tilde{x})}{m (\tilde{x})} \right) \right] \]  

(60)

has never been reported elsewhere in the literature. Therefore, one should cast the PDM Schrödinger equation as

\[ \left\{ \frac{\hat{P}_j (\tilde{x})}{\sqrt{m (\tilde{x})}} \right\}^2 + V (\tilde{x}) \phi (\tilde{x}) = E \phi (\tilde{x}), \quad \text{OR} \quad \left\{ \hat{x}_j^2 (\tilde{x}) + V (\tilde{x}) \right\} \phi (\tilde{x}) = E \phi (\tilde{x}). \]  

(61)

This would, in effect, fix the ordering ambiguity problem in the von Roos Hamiltonian (1) that has been known in the literature for few decades. Therefore, only under our especial type of point transformation settings that the PDM
classical and quantum mechanical correspondence as well as the construction of the PDM-momentum (operator) were made feasible.

On the electromagnetic interactions side, moreover, it was very vital to start again (in section IV) from the classical mechanical settings to find out the corresponding quantum mechanical settings (using the appropriate PDM pseudo-momentum (operator) forms) and dwell on the transformational nature of the minimal coupling. We have observed that for the PDM classical Hamiltonian in (23) one may simply use the minimal coupling

\[ \pi_j (\vec{x}) \to \pi_j (\vec{x}) - e A_j (\vec{x}) \quad \text{and} \quad E = H_{\text{classical}} \to E - e \varphi (\vec{x}) \]  

(62)

to incorporate electromagnetic interactions. Likewise, in quantum mechanics, for the PDM-Schrödinger equation (22) one uses the minimal coupling

\[ \hat{\pi}_j (\vec{x}) \to \hat{\pi}_j (\vec{x}) - e A_j (\vec{x}) \quad \text{and} \quad E \to E - e \varphi (\vec{x}). \]  

(63)

Which, in fact, looks very much like a textbook minimal coupling but with the classical PDM pseudo-momentum \( \pi_j (\vec{x}) \) and the quantum PDM pseudo-momentum operator \( \hat{\pi}_j (\vec{x}) \) rather than the momentum \( p_j = m_o \dot{x}_j \) and momentum operator \( \hat{p}_j = -i \partial / \partial x \), respectively. This result renders Dutra and Oliveira’s [10] approach to this problem inappropriate (as documented in our discussion following (34) of section IV). Of course, such minimal coupling (63) does not hold true for Klein-Gordon and Dirac relativistic wave equations. The PDM concept fits very well without any ambiguity conflict into Klein-Gordon and Dirac equations (see [52–54] for more details on this issue). Moreover, two vector potentials that satisfy the Coulomb gauge \( \partial \theta_j A_j (\vec{q}) = 0 \) are used (in section V) as illustrative examples, \( \vec{A} (\vec{q}) = B_o (-q_2, 0, 0) \) and \( \vec{A} (\vec{q}) = B_o (-q_2, q_1, 0)/2 \). The mapping between the constant mass settings and PDM settings along with their isospectrality is made clear (in section V).

Finally, although our methodical proposal above is introduced to deal with a three-dimensional PDM-Schrödinger equation, it is also feasibly applicable to a more commonly used two-dimensional problems (c.f., e.g. Dutra and Oliveira [10] or Correa et al. [2] and related references therein). However, the three-dimensional case is a more general and instructive one.
