A quasi-free position-dependent mass jump and self-scattering correspondence

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Abstract

A quasi-free quantum particle endowed with a Heaviside position-dependent mass jump is observed to experience scattering effects manifested by its by-product introduction of the derivative of the Dirac delta point dipole interaction, δ′(x) = δ, δ(x). Using proper parametric mappings, the reflection and transmission coefficients are obtained. A new ordering ambiguity parameter set is reported.

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1. Introduction

Hamiltonians for particles endowed with position-dependent mass (PDM) (i.e. \(M(x) = m, m(x)\)) have attracted much research attention over the last few decades [1–29]. Such attention was inspired not only by the feasible applicability of PDM settings to the study of various physical problems (e.g. the many-body problem, semiconductors, quantum dots and quantum liquids) but also by the mathematical challenge associated with the ordering ambiguity in the PDM van Roos Hamiltonian. The non-commutativity between the momentum operator (with \(\hbar = m = 1\) unit) \(\hat{p}_x = -i\hat{\partial}_x\) and the PDM resulted in an ordering ambiguity in the non-uniqueness representation of the kinetic energy operator

\[ T = -\frac{1}{2} \left[ M(x)^a \partial_x M(x)^b \partial_x M(x)^c \right] \]

where \(\alpha, \beta,\) and \(\gamma\) are called the van Roos ordering ambiguity parameters satisfying the van Roos constraint \(\alpha + \beta + \gamma = -1\) (cf e.g. [25–29]).

In the literature, there exist several suggestions on the van Roos ordering ambiguity parameters. Among them are Gora and Williams’ (\(\beta = \gamma = 0, \alpha = -1\)), Ben Daniel and Duke’s (\(\alpha = \gamma = 0, \beta = -1\)), Zhu and Kroemer’s (\(\alpha = \gamma = -1/2, \beta = 0\)), Li and Kuhn’s (\(\beta = \gamma = -1/2, \alpha = 0\)) and the very recent Mustafa and Mazharimousavi’s (\(\alpha = \gamma = -1/4, \beta = -1/2\)) (cf e.g. [10, 29] for more details of this issue). However, the continuity conditions at the abrupt heterojunction between two crystals imply that \(\alpha = \gamma\); otherwise for \(\alpha \neq \gamma\) the wavefunctions vanish at the boundaries and the heterojunction therefore plays the role of an impenetrable barrier (cf e.g. Mustafa and Mazharimousavi [10] and Koc et al [28]). Moreover, if we add this to de Souza Dutra and Almeida’s [9] reliability test, then the number of acceptable ordering-ambiguity parametric values reduces to two sets: the Zhu and Kroemer (\(\alpha = \gamma = -1/2, \beta = 0\)) and Mustafa and Mazharimousavi (\(\alpha = \gamma = -1/4, \beta = -1/2\)) sets. Nevertheless, it has been observed (cf e.g. [29]) that the physical and/or mathematical admissibility of a given ambiguity parameter set depends not only on the continuity conditions at the abrupt heterojunction boundaries and/or Dutra and Almeida’s [9] reliability test. The PDM and/or potential forms have their signature in the process. Therefore, the general consensus is that there is no unique choice for these ambiguity parameters.

On the other hand, research activities on the analysis of the one-dimensional Hamiltonians associated with the so-called ‘point’ or ‘contact’ interactions (i.e. zero everywhere except at the origin \(x = 0\), similar to the Dirac delta \(\delta(x)\) distribution), in solid-state physics, were stimulated by a rapid progress in the fabrication of nanoscale quantum devices [30–36]. Such interactions are intuitively understood as sharply localized potentials exhibiting a number of interesting features. Their applicability extends to optics when electromagnetic waves scatter at the boundaries of thin layers in dielectric media [37].

Within the context of the recent interest in exactly solvable one-dimensional Schrödinger models of scattering accompanied by PDM particles, we consider a free particle (i.e. subjected to \(V(x) = 0\) potential) endowed with a
Heaviside mass function/distribution of the form
\[ m(x) = 1 + \mu h(x); \quad \mathbb{R} \ni \mu > 0, \tag{1} \]
where
\[ h(x) = \frac{1 + \text{sgn}(x)}{2} = \begin{cases} 0, & x < 0, \\ 1/2, & x = 0, \\ 1, & x > 0 \end{cases} \]
is the discontinuous Heaviside step function. Nevertheless, for the convenience of the present study, we shall use a more general form for the PDM function to read
\[ m(x) = f(h(x)) = \begin{cases} m_1, & x < 0, \\ m_2, & x = 0, \\ m_3, & x > 0 \end{cases} \tag{2} \]
Of course this would practically refer to ‘PDM jumps’ (cf e.g. [38–40]). To the best of our knowledge, such unusual PDM settings of discontinuous functional nature have been discussed in the literature (cf e.g. [38–40]), but never within our present methodical proposal.

The organization of this paper is as follows. In section 2, we show that a quasi-free quantum particle (i.e. subjected to \( V(x) = 0 \), whereas \( V_{\text{eff}}(q(x)) \neq 0 \)) endowed with the Heaviside PDM of (2) experiences scattering effects. Upon implementing a point canonical transformation (PCT) recipe, the derivative of the Dirac delta distribution turns out to form the effective potential (i.e. \( V_{\text{eff}}(q(x)) \sim \delta'(x) \)). As a result, a scattering problem is obtained in the process (and the notion of self-scattering correspondence is unavoidable therefore). The detailed solution of it can be inferred from the scattering potential \( V(q) = -a\delta(q) + b\delta'(q) \) of Gadella et al [36] (using proper parametric mappings to our model, of course). See [36] for the mathematical and/or physical details. Moreover, a new ordering ambiguity parameter set is obtained as the only feasible set to admit. Our concluding remarks are given in section 3.

2. PCT recipe and self-scattering correspondence

Under PDM settings, the Schrödinger equation for a free PDM quantum particle, \( V(x) = 0 \), [22–29] reads
\[ \left[ -\frac{1}{2} \frac{\partial^2}{\partial t^2} \left( \frac{1}{m(x)} \right) \partial_x + \tilde{V}(x) \right] \psi(x) = E \psi(x), \tag{3} \]
with
\[ \tilde{V}(x) = g_1 \frac{m''(x)}{m(x)^2} - g_2 \frac{m'(x)^2}{m(x)^3}, \tag{4} \]
where primes denote derivatives with respect to \( x \) and
\[ g_1 = \frac{1}{8} \left( 1 + \beta \right); \quad g_2 = \frac{1}{8} \left[ a \left( \alpha + \beta + 1 \right) + \beta + \frac{9}{16} \right]. \tag{5} \]
We now follow the well-known PCT recipe (cf e.g. [19]) through the substitution of \( \psi(x) = m(x)^{1/4} \phi(q(x)) \) in (3) to imply (with \( q(x) = \sqrt{m(x)} \))
\[ q(x) = \int x \sqrt{m(t)} dt = \int x \sqrt{f(h(t))} dt = \sqrt{x} \sqrt{f(h(x))} \tag{6} \]
and obtain a Schrödinger equation of the form
\[ \left[ -\frac{1}{2} \frac{\partial^2}{\partial y^2} + V_{\text{eff}}(q) \right] \phi(q) = E \phi(q), \tag{7} \]
where
\[ V_{\text{eff}}(q) = \tilde{V}(x) + \frac{7m'(x)^2}{2m(x)^2} - \frac{m''(x)}{8m(x)^2}. \tag{8} \]
Equation (8), with \( m(x) = f(h(x)) \), \( m'(x) = \partial_x m(x) \) and \( f'(h(x)) = \partial_{h(x)} f(h(x)) \), yields
\[ V_{\text{eff}}(q(x)) = G_1 \frac{m''(x)}{m(x)^2} - G_2 \frac{m'(x)^2}{m(x)^3} = G_1 \frac{\delta'(h(x))}{f(h(x))} + \frac{\delta(x)^2}{f'(h(x))} \times \left( G_1 \frac{f''(h(x))}{f'(h(x))^2} - G_2 \frac{f'(h(x))}{f'(h(x))} \right), \tag{9} \]
with
\[ G_1 = \frac{1}{8} \left( 1 + 2 \beta \right); \quad G_2 = \frac{1}{8} \left[ a \left( \alpha + \beta + 1 \right) + \beta + \frac{9}{16} \right]. \tag{10} \]
where \( \delta(x) \) denotes the Dirac delta function and \( \delta'(x) = \partial_x \delta(x) \) is the derivative of the Dirac delta function. Hereby, it is obvious that the \( h(x) \)-dependent terms associated with \( \delta'(x) \) and \( \delta(x)^2 \) form continuous functions except at the origin \( x = 0 \). They are thus functions of a finite discontinuity. In this case, we may benefit from the well-known definitions associated with the Dirac delta distributions (cf e.g. equations (4) and (5) of [36]). That is, if we take
\[ U(x) = \frac{f'(h(x))}{f(h(x))^2} \]
as a discontinuous function of \( x \), then the distributions \( U(x)\delta(x) \) and \( U(x)\delta'(x) \) can be rewritten as
\[ U(x)\delta(x) = U(0)\delta(x), \tag{11} \]
\[ U(x)\delta'(x) = U(0)\delta'(x) - U'(0)\delta(x). \tag{12} \]
This would, in turn, imply that the effective potential in (9) can be recast as
\[ V_{\text{eff}}(q(x)) = G_1 U(0)\delta'(x) + (2G_1 - G_2) \frac{f'(h(x))}{f(h(x))^2} \delta(x)^2. \tag{13} \]
However, to avoid the physical and/or mathematical meaninglessness of \( \delta(x)^2 \), two feasible solutions for (13) are obtained. The simplest of them is achieved by taking \( G_1 = 0 \) and \( G_2 = 0 \) (i.e. Mustafa and Mazharimousavi’s [10] (MM), ordering ambiguity parameters \( \alpha = \gamma = -1/4 \) and \( \beta = -1/2 \). In this case, the Heaviside position-dependent particle at hand (2) remains free and admits a free-particle solution therefore. However, the triviality of such a choice (i.e. \( G_1 = 0 = G_2 \)) inspires the search for yet another feasible solution where \( G_1 \neq 0 \) (i.e. \( \beta \neq -1/2 \)).

If we just recollect that \( \alpha + \beta + \gamma = -1 \) (i.e. the von Roos constraint) and impose the continuity conditions at
the abrupt heterojunction boundaries (i.e. simply \( \alpha = \gamma \)), a manifesto that ensures the continuity of \( m(x)\phi(x) \) and \( m(x)\psi(x) \) at the heterojunction boundaries (along with the choice of \( 2G_1 - G_2 = 0 \)), we would then dismiss the \( \delta(x)^2 \) ambiguity. Under such conditions, a new set of ordering ambiguity parameters (the only admissible parametric set within the current methodical proposal, labeled as MM1-ordering hereinafter) that casts \( \alpha = \gamma = -3/4 \) and \( \beta = 1/2 \) is obtained. As such and within this new set of ambiguity parameters, the effective potential (13) collapses into a simple form

\[
V_{\text{eff}}(q(x)) = \frac{U(0)}{2} \delta(x); \quad U(x) = \frac{f'(h(x))}{f(h(x))^2}.
\]

We clearly observe that a scattering problem of a quasi-free quantum particle (i.e. \( V(x) = 0 \), whereas \( V_{\text{eff}}(q(x)) \neq 0 \)) subjected to the derivative of the Dirac delta interaction (also called the point dipole interaction) is manifested by (14) of Hamiltonian (7). The detailed solution of it can be inferred from the scattering coefficients of the \( V(q) = -a\delta(q) + b\delta'(q) \) potential of Gadella et al [36] by taking \( m = 1, a = 0 \) and \( b = U(0)/2 \) as proper parametric mappings to our model. Choosing to skip all the mathematical and/or physical details, the reflection and transmission coefficients (see equation (23) of [36]) would, respectively, read

\[
R = \frac{-4U(0)}{4 + U(0)^2}
\]

and

\[
T = \frac{4 - U(0)^2}{4 + U(0)^2}.
\]

In a straightforward manner, it can be easily shown that the condition \( |R|^2 + |T|^2 = 1 \) is satisfied. Consequently, a free quantum particle endowed with the PDM setting of (2) may experience scattering effects. Moreover, it is obvious that while \( U(0) = 0 \) yields (although trivial) a totally transparent/reflectionless derivative of the Dirac delta scatterer, \( U(0) = \pm 2 \) yields a totally reflective one.

In due course, the PDM jump of (1) implies

\[
q(x) = x \sqrt{f(h(x))} = x [1 + \mu h(x)]
\]

and

\[
U(x) = \frac{\mu}{1 + \mu h(x)} \implies U(0) = \frac{\mu}{1 + \mu/2}.
\]

In a straightforward manner, however, one may substitute \( U(0) \) into (18) to obtain the transmission and reflection coefficients (15) and (16), respectively, as

\[
R = \frac{-4\mu(1 + \mu/2)^2}{4(1 + \mu/2)^4 + \mu^2}
\]

and

\[
T = \frac{4(1 + \mu/2)^2 - \mu^2}{4(1 + \mu/2)^4 + \mu^2}.
\]

Asymptotically speaking, the Taylor series expansions about \( \mu \to 0 \) (i.e. \( 0 < \mu \ll 1 \), also very likely to be experimentally applicable) would result in casting the reflection and transmission intensities, respectively, as \( |R|^2 \approx \mu^2 + O(\mu^3) \) and \( |T|^2 \approx 1 - \mu^2 + O(\mu^3) \). Within such asymptotic tendencies, it is obvious that increasing the value of \( \mu \) from just above 0 to 1 would make the derivative of the Dirac delta scatterer less transparent until total reflection is obtained when \( \mu = 1 \).

3. Concluding remarks

In this work, we have considered a quasi-free quantum particle (i.e. \( V(x) = 0 \), whereas \( V_{\text{eff}}(q(x)) \neq 0 \)) endowed with the Heaviside PDM jump in (1). Using PCT, we have encountered a physically and/or mathematically ambiguous \( \delta(x)^2 \) term in (13). To remove this ambiguity, two possible ordering ambiguity parametric sets are obtained. The first of them is the MM-ordering ambiguity parameterization [10], i.e. \( \alpha = \gamma = -1/4 \) and \( \beta = -1/2 \), which leaves our quasi-free PDM particle in (1) as free (i.e. it admits the regular textbook free particle solution). However, it is only under a specific (although rather new) set of ordering ambiguity parameterization (i.e. \( \alpha = \gamma = -3/4 \) and \( \beta = 1/2 \)) that our PDM particle in (1) introduces the derivative of Dirac delta distribution/function, \( \delta'(x) \), manifesting, in effect, a scattering problem. We were able to obtain the related reflection (15) and transmission (16) coefficients for any \( U(0) \) of \( U(x) \) in (14). Moreover, we have predicted that our quasi-free PDM particle may totally reflect itself (documented in (17)–(20)) by the effective potential it introduces (i.e. the derivative of the Dirac delta function, \( \delta'(x) \), in this case).

Nevertheless, should our PDM quantum particle (1) be also subjected to the Dirac delta potential \( V(x) = -a\delta(x) \) (that appears in equation (1) of Gadella et al [36], though readily lays far beyond our methodical proposal above), then the reflection and transmission coefficients would, respectively, read

\[
R = \frac{-4[a + ikU(0)]}{4a + ik[4 + U(0)^2]}
\]

and

\[
T = \frac{ik[4 - U(0)^2]}{4a + ik[4 + U(0)^2]}.
\]

The comprehensive discussion of this is given by Gadella et al [36].

We have very recently shown (see [29] for more details) that the ordering ambiguity conflict (associated with the non-unique representation of the von Roos Hamiltonian), of which ordering would be the best representative for the PDM Hamiltonian, cannot be resolved within the abrupt heterojunction boundary conditions and the Dutra and Almeida [9] reliability test. The PDM and the potential forms have their say in the process. The current Heaviside PDM jump (2) is not just an interesting example but also an additional documentation of this observation.

Finally, the reader may wish to consult Lévy-Leblond [41] (and related references cited therein) for more details on the issue of consistency and usefulness of the PDM Schrodinger equation. Therein, the authors work was devoted to sustaining and strengthening the conclusions that not only the use of PDM give correct approximation...
but also a conceptually consistent approach. In fact, the kinetic energy operator in the PDM Hamiltonian of (3) is an interesting problem with many aspects that are yet to be explored (cf e.g. Mustafa [42]).

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