

Brazilian Journal of Physics ISSN: 0103-9733 luizno.bjp@gmail.com

Sociedade Brasileira de Física Brasil

Nobre, F. D.; Rego-Monteiro, M. A.

Non-Hermitian PT Symmetric Hamiltonian with Position-Dependent Masses: Associated Schrödinger

Equation and Finite-Norm Solutions

Brazilian Journal of Physics, vol. 45, núm. 1, 2015, pp. 79-88

Sociedade Brasileira de Física

Sâo Paulo, Brasil

Available in: http://www.redalyc.org/articulo.oa?id=46433753012



Complete issue

More information about this article

Journal's homepage in redalyc.org



Scientific Information System

Network of Scientific Journals from Latin America, the Caribbean, Spain and Portugal Non-profit academic project, developed under the open access initiative

#### **STATISTICAL**



# Non-Hermitian PT Symmetric Hamiltonian with Position-Dependent Masses: Associated Schrödinger Equation and Finite-Norm Solutions

F. D. Nobre · M. A. Rego-Monteiro

Received: 23 July 2014 / Published online: 7 November 2014 © Sociedade Brasileira de Física 2014

**Abstract** A one-dimensional non-Hermitian PT symmetric Hamiltonian, characterized by position-dependent masses, defines a Schrödinger equation in terms of a field  $\Psi(x,t)$ . Based on an exact classical field theory, the necessity of an extra field  $\Phi(x,t)$  (which satisfies a conjugate equation and in general different is from  $\Psi^*(x,t)$ ) is shown. Simple applications are investigated by solving analytically both equations and it is shown that the effective masses proposed lead to a probability density characterized by a finite norm, typical of the physical situation that occurs with the concentration of electrons in some semiconductor heterojunctions. An extension to a three-dimensional space is also presented.

**Keywords** Non-homogeneous Schrödinger equation · Non-hermitian hamiltonian · Solutions of wave equations · Localized states · Classical field theory · Non-extensive thermostatistics

#### 1 Introduction

e-mail: fdnobre@cbpf.br

Quantum mechanics represents one of the most successful theories in physics, leading to an appropriate description of an incredibly amount of physical phenomena [1]. However, many of its fundamental concepts are often remote from our daily experience, such as the single plane-wave solution, used for representing a free particle. Since this

F. D. Nobre (⋈) · M. A. Rego-Monteiro Centro Brasileiro de Pesquisas Físicas, National Institute of Science and Technology for Complex Systems, Rua Xavier Sigaud 150, 22290-180 Rio de Janeiro, RJ, Brazil solution presents a nonzero amplitude over all space, its norm diverges, so that it is not appropriate for describing wave pulses of wave trains. However, the linear aspect of the Schrödinger equation (SE) ensures that one can add many solutions such as to still have a solution. In this way, a localized solution may be constructed by defining a superposition of plane waves, i.e., a Fourier series, leading to the so-called wave-packet concept.

Proposals for overcoming the above-mentioned difficulty, and also motivated by an adequate understanding of several phenomena related to complex systems, have appeared in the latest years, based on modifications of the SE. For this purpose, attempts have occurred, and one of them consists in turning the SE into a nonlinear equation. In this case, one should mention two schemes: (i) Introduction of an extra cubic term in the wave function that becomes responsible for the modulation of some particular type of solution [2, 3]; (ii) modification of exponents of existing linear terms. This second scheme was applied in Refs. [4–7], and it is currently employed within non-extensive statistical mechanics [8]. As immediate consequences, analytical treatments may become hard, in such a way that simple properties in the linear case, like conservation of probability by means of a continuity equation, may become rather nontrivial subjects (see, e.g., Refs. [5, 7]). Hence, very frequently, one has to make use of numerical procedures, so that the latest advances in computer technology have stimulated the study of generalized equations, leading to considerable progresses. Particularly, many areas of physics have benefited from such studies, like nonlinear optics, superconductivity, plasma physics, and non-equilibrium statistical mechanics.

Although nonlinear equations may be suitable for describing many natural phenomena, other physical



systems, e.g., those associated with non-homogeneous media, may require equations characterized by position-dependent coefficients; in several cases, one may still keep the linear character of such equations. This happens to be the case in the proposals of Refs. [9–17], which considered linear SEs, but with position-dependent masses. One main motivation concerns a proper description of some semiconductor heterostructures [18, 19].

Very frequently, within the context of nonlinear and/or nonhomogeneous SEs, one has to deal with non-Hermitian Hamiltonians [20]. Nowadays, it is known that hermiticity is not a necessary condition for a consistent quantum theory, since it has been demonstrated in the literature that non-Hermitian Hamiltonians may also present real energy eigenvalues, leading to a well-defined quantum theory [14, 17, 20–27]. Particularly, among the non-Hermitian Hamiltonians, a great interest has been dedicated to those characterized by a PT symmetry, i.e., symmetric under both P (parity, or space-reflection operator, which reverses position and momentum,  $x \rightarrow -x$ ,  $p \rightarrow -p$ ) and T (time reversal operator, which reverses time and momentum,  $t \to -t$ ,  $p \rightarrow -p$ , also requiring the reverse of the sign of the complex number,  $i \rightarrow -i$ ). Hence, the resulting PT operation changes  $x \to -x$ ,  $t \to -t$ , and  $i \to -i$ . Recently, an alternative formulation of quantum mechanics has appeared, in which the requirement of Hermiticity of the Hamiltonian  $\hat{H}$ was replaced by the condition of space-time reflection; consequently, if H presents an unbroken PT symmetry, then its associated energy spectrum should be real [20, 22–27].

Another fundamental issue when dealing with non-Hermitian Hamiltonians concerns the positivity and finiteness of the norm of states. Eventually, one may end up with states leading to a negative norm, which prevents its use in the probabilistic interpretation of quantum mechanics. In some of these cases, an operator has been introduced (called C operator), in terms of which a time-independent inner product is constructed, yielding a positive-definite norm. Essentially, the operator C contributes with a factor -1 whenever it acts on states with negative norm [20].

In the present work, we introduce a one-dimensional non-Hermitian PT symmetric Hamiltonian  $\hat{H}$ , characterized by position-dependent masses, which defines a Schrödinger equation associated with the field  $\Psi(x,t)$ . By applying an exact classical field theory, we show that one needs to introduce an extra field  $\Phi(x,t)$  for consistency; this field satisfies a conjugate equation, written in terms of the Hamiltonian conjugate  $\hat{H}^{\dagger}$ . In the next section, we define the Hamiltonian and its associated Schrödinger equation, characterized by a particular form for the position-dependent masses. It is argued that the dependence introduced herein might be relevant for physical systems presenting interfaces along which the chemical composition varies, like in semiconductor heterostructures, where such changes do not

occur abruptly, but instead, they are graded over some specified distance, and consequently, the effective mass becomes a continuous function of the position. In the present proposal, the particular form of mass dependence leads to a maximum probability density at the origin, decreasing continuously away from the origin, representing typically the physical situation that occurs with the concentration of electrons in pnp junctions. Hence, a classical field theory is constructed, by introducing a Lagrangian density, in such a way to obtain the Schrödinger equation, as well as its conjugate equation, associated with the extra field. Moreover, defining an appropriate probability density in terms of the two fields, the continuity equation is demonstrated. In Section 3, we consider two simple applications, namely, the free particle in open space and the particle confined in an infinite square well  $(-L \le x \le L)$ , solving analytically the equations for the fields  $\Psi(x, t)$  and  $\Phi(x, t)$ . We show that the energy spectrum is quantized in both applications, and more interestingly, that the free-particle solution presents a finite norm in full open space. In Section 4, a three-dimensional proposal is also presented, in terms of the two fields  $\Psi(\vec{x}, t)$  and  $\Phi(\vec{x}, t)$ ; it is shown that all results obtained in the one-dimensional analysis may be extended to three dimensions. Finally, in Section 5, we present our conclusions.

## 2 The Hamiltonian and Its Conjugate

Let us consider the following SE,

$$i\hbar \frac{\partial \Psi(x,t)}{\partial t} = -\frac{\hbar^2}{2m} \hat{D}_{\gamma}^2 \Psi(x,t) + V(x)\Psi(x,t)$$
$$\left(\hat{D}_{\gamma} = (1+\gamma x^2) \frac{\partial}{\partial x}\right), \tag{1}$$

where V(x) denotes a potential and  $\hat{D}_{\gamma}$  is a deformed derivative in space [28]. This equation may be written also in terms of a one-dimensional, non-Hermitian PT symmetric Hamiltonian  $\hat{H}$ ,

$$i\hbar \frac{\partial \Psi(x,t)}{\partial t} = \hat{H}\Psi(x,t) ,$$
 (2)

where

$$\hat{H} = -\frac{\hbar^2}{2m_e} \frac{\partial^2}{\partial x^2} - \frac{\hbar^2}{4} \left[ \frac{d}{dx} \left( \frac{1}{m_e} \right) \right] \frac{\partial}{\partial x} + V(x)$$

$$\left( m_e = \frac{m}{\left( 1 + \gamma x^2 \right)^2} \right). \tag{3}$$

The above Hamiltonian is characterized by position-dependent masses,  $m_e \equiv m_e(x)$ , interpreted as the particle's position-dependent effective mass, found in real systems, like in semiconductors of nonuniform chemical composition



[9], and semiconductor heterostructures [18, 19]. In the definition above for  $m_e$ ,  $\gamma$  represents a real non-negative parameter (with dimensions  $[L]^{-2}$ ) that may vary according to the physical system considered; moreover,  $m_e$  follows parity symmetry,  $x \to -x$ , which should also be obeyed by the potential, i.e., V(-x) = V(x).

A heterostructure is defined as a semiconductor structure in which the chemical composition changes with position; hence, an electron moving in such a structure presents an effective mass that varies with its position. The simplest heterostructure consists of a single heterojunction, represented by an interface across which the chemical composition changes. Usually, a heterojunction is made between two materials for which there exists a continuum of solid solutions, so that the chemical variation does not occur abruptly, but instead, it drops continuously with the position, and consequently, leading to a similar behavior for the effective mass. Such heterojunctions present desirable properties for some applications. The proposal for an effective mass  $m_e =$  $m/(1+\gamma x)^2$ , considered in Refs. [14–17], is expected to be relevant for a some types of np junctions, where a gradual decrease in the concentration of electrons is verified for x > 0. In the present framework, the effective-mass form of (3) is symmetric around its maximum value at x = 0 and decreases for increasing values of |x|, so that  $m_e \sim |x|^{-4}$ , when  $\sqrt{\gamma}x \gg 1$ . Hence, this proposal should be applicable for pnp junctions, where the parameter  $\gamma$  would depend on the particular types of materials used in the associated junctions.

Recently, it was shown that for some class of Schrödinger equations, defined in terms of non-Hermitian Hamiltonians [like the one of (3)], one needs to deal with an extra equation assigned to the Hermitian conjugate of the corresponding Hamiltonian [5, 7, 17]. Herein, we follow closely the procedure carried in Ref. [17], where a classical-field theory was developed by introducing a Lagrangian density,  $\mathcal{L}$ , depending on two dimensionless fields  $\Psi(x,t)$  and  $\Phi(x,t)$ , on their time derivatives, as well as spatial derivatives,

$$\mathcal{L} \equiv \mathcal{L}\left(\Psi, \partial_x \Psi, \partial_x^2 \Psi, \partial_t \Psi, \Phi, \partial_x \Phi, \partial_t \Phi, \Psi^*, \partial_x \Psi^*, \partial_x^2 \Psi^*, \partial_t \Psi^*, \Phi^*, \partial_x \Phi^*, \partial_t \Phi^*\right), \tag{4}$$

with  $\partial_x \equiv \partial/\partial x$ ,  $\partial_x^2 \equiv \partial^2/\partial x^2$ , and  $\partial_t \equiv \partial/\partial t$ . One should call the attention to the fact that the Lagrangian density defined above presents a dependence up to first spatial derivative in the field  $\Phi(x,t)$  and up to the second one in the field  $\Psi(x,t)$ ; this represents an important requirement for obtaining the correct Euler-Lagrange equations for these two fields [29, 30]. Therefore, in the first case, one has a

standard Euler-Lagrange equation

$$\frac{\partial \mathcal{L}}{\partial \Phi} - \partial_x \left[ \frac{\partial \mathcal{L}}{\partial (\partial_x \Phi)} \right] - \partial_t \left[ \frac{\partial \mathcal{L}}{\partial (\partial_t \Phi)} \right] = 0 , \qquad (5)$$

whereas in the later, one should take into account the contribution from its second-derivative term

$$\frac{\partial \mathcal{L}}{\partial \Psi} - \partial_x \left[ \frac{\partial \mathcal{L}}{\partial (\partial_x \Psi)} \right] - \partial_t \left[ \frac{\partial \mathcal{L}}{\partial (\partial_t \Psi)} \right] + \partial_x^2 \left[ \frac{\partial \mathcal{L}}{\partial (\partial_x^2 \Psi)} \right] = 0.$$
(6)

Herein, we propose the following Lagrangian density

$$\mathcal{L} = \frac{i\hbar}{2} \Phi(x,t)\partial_t \Psi(x,t) + \frac{\hbar^2}{8} \left[ \frac{d}{dx} \left( \frac{1}{m_e} \right) \right] \Phi(x,t)\partial_x \Psi(x,t)$$

$$+ \frac{\hbar^2}{4m_e} \Phi(x,t) \partial_x^2 \Psi(x,t) - \frac{1}{2} V(x) \Psi(x,t) \Phi(x,t)$$

$$- \frac{i\hbar}{2} \Phi^*(x,t)\partial_t \Psi^*(x,t) + \frac{\hbar^2}{8} \left[ \frac{d}{dx} \left( \frac{1}{m_e} \right) \right] \Phi^*(x,t)\partial_x \Psi^*(x,t)$$

$$+ \frac{\hbar^2}{4m_e} \Phi^*(x,t) \partial_x^2 \Psi^*(x,t) - \frac{1}{2} V(x) \Psi^*(x,t) \Phi^*(x,t) , \qquad (7)$$

which will be shown to be appropriate in what follows. Substituting the above Lagrangian density in (5), one obtains the SE of (2); furthermore, the Euler-Lagrange equation of (6) leads to the equation for the field  $\Phi(x, t)$ ,

$$-i\hbar \frac{\partial \Phi(x,t)}{\partial t} = \hat{H}^{\dagger} \Phi(x,t) , \qquad (8)$$

where  $\hat{H}^{\dagger}$  is the Hermitian conjugate of the Hamiltonian operator defined in (2). One has that

$$\hat{H}^{\dagger} = -\frac{\hbar^2}{2m_e} \frac{\partial^2}{\partial x^2} - \frac{3\hbar^2}{4} \left[ \frac{d}{dx} \left( \frac{1}{m_e} \right) \right] \frac{\partial}{\partial x} - \frac{\hbar^2}{4} \left[ \frac{d^2}{dx^2} \left( \frac{1}{m_e} \right) \right] + V(x) . \tag{9}$$

One should notice that only for a constant mass,  $m_e = m$  (i.e.,  $\gamma = 0$ ), is that one has a Hermitian Hamiltonian,  $\hat{H}^{\dagger} = \hat{H}$ , and (2) and (8) are related by a conjugate operation, with  $\Phi(x,t) = \Psi^*(x,t)$ . For  $\gamma > 0$ , these two equations are not simply related, so that both Hamiltonians and fields should be considered in a complete analysis. Indeed,  $\gamma$  represents a deformation parameter, associated with the non-Hermiticity of the Hamiltonian operator, in the sense that  $\hat{H}^{\dagger} \neq \hat{H}$ , if  $\gamma > 0$ , whereas Hermiticity is recovered for  $\gamma = 0$ . One should notice the close analogy with nonextensive statistical mechanics [8]; in fact, the Hamiltonian  $\hat{H}$  of (2) and (3) was originally based on a deformed-derivative operator, which was shown to be very useful for performing calculations in such a theory [28].



Considering these two fields, one can define a probability density

$$\rho(x,t) = \frac{1}{2} \left[ \Psi(x,t) \Phi(x,t) + \Psi^*(x,t) \Phi^*(x,t) \right]. \tag{10}$$

The consistency of the procedure above is reinforced by the continuity equation

$$\frac{\partial \rho(x,t)}{\partial t} + \frac{\partial j(x,t)}{\partial x} = 0, \qquad (11)$$

where the current density is given by

$$j(x,t) = -\frac{\hbar}{4i} \left\{ \frac{\partial}{\partial x} \left[ \frac{\Phi(x,t)}{m_e} \right] \Psi(x,t) - \frac{\Phi(x,t)}{m_e} \frac{\partial \Psi(x,t)}{\partial x} - \frac{1}{2} \left[ \frac{d}{dx} \left( \frac{1}{m_e} \right) \right] \Phi(x,t) \Psi(x,t) - \frac{\partial}{\partial x} \left[ \frac{\Phi^*(x,t)}{m_e} \right] \Psi^*(x,t) + \frac{\Phi^*(x,t)}{m_e} \frac{\partial \Psi^*(x,t)}{\partial x} + \frac{1}{2} \left[ \frac{d}{dx} \left( \frac{1}{m_e} \right) \right] \Phi^*(x,t) \Psi^*(x,t) \right\}.$$
(12)

It should be mentioned that (11) holds for general  $m_e(x)$  and V(x), ensuring the conservation of probability for all times. In order to achieve continuity, the introduction of the extra field  $\Phi(x, t)$  and its associated equation [(8)] becomes essential; this result is not possible by considering only the SE of (2) and its complex conjugate.

Based on the above results, we define the inner product involving these two fields

$$(\Psi(x,t),\Phi(x,t)) = \frac{1}{2} \int_{-\infty}^{\infty} dx \left[ \Psi(x,t)\Phi(x,t) + \Psi^*(x,t)\Phi^*(x,t) \right]$$
$$= \int_{-\infty}^{\infty} dx \, \rho(x) , \qquad (13)$$

so that, by definition

$$(\Psi(x,t), \Phi(x,t))^* = (\Psi(x,t), \Phi(x,t)). \tag{14}$$

Now, (2) and (8) indicate that  $\Psi(x,t)$  and  $\Phi(x,t)$  should be the right and left wavefunctions of  $\hat{H}$ , respectively, whereas the order should be inverted for  $\hat{H}^{\dagger}$ . In this way, one can write the expectation values,

$$\langle \hat{H} \rangle = \frac{1}{2} \int_{-\infty}^{\infty} dx \, \Phi(x, t) \hat{H} \Psi(x, t) + \frac{1}{2} \left[ \int_{-\infty}^{\infty} dx \, \Phi(x, t) \hat{H} \Psi(x, t) \right]^{*}$$

$$= \frac{1}{2} \int_{-\infty}^{\infty} dx \, \Phi(x, t) \hat{H} \Psi(x, t) + \frac{1}{2} \int_{-\infty}^{\infty} dx \, \Phi^{*}(x, t) \left[ \hat{H} \Psi(x, t) \right]^{*}$$

$$= \frac{i\hbar}{2} \int_{-\infty}^{\infty} dx \, \left[ \Phi(x, t) \, \frac{\partial \Psi(x, t)}{\partial t} - \Phi^{*}(x, t) \, \frac{\partial \Psi^{*}(x, t)}{\partial t} \right], \qquad (15)$$

as well as,

$$\langle \hat{H}^{\dagger} \rangle = \frac{1}{2} \int_{-\infty}^{\infty} dx \ \Psi(x,t) \hat{H}^{\dagger} \Phi(x,t) + \frac{1}{2} \left[ \int_{-\infty}^{\infty} dx \ \Psi(x,t) \hat{H}^{\dagger} \Phi(x,t) \right]^{*}$$

$$= \frac{i\hbar}{2} \int_{-\infty}^{\infty} dx \left[ \Psi^{*}(x,t) \frac{\partial \Phi^{*}(x,t)}{\partial t} - \Psi(x,t) \frac{\partial \Phi(x,t)}{\partial t} \right]. \tag{16}$$

Therefore, in general, one has that  $\langle \hat{H} \rangle \neq \langle \hat{H}^{\dagger} \rangle$ , whereas these expectation values become equal only in the limit  $\gamma=0$ . In what follows, we will show that, considering a particular stationary-state solution, the standard procedure for finding the adjoint of a differential operator by means of integrations by parts, and using appropriate boundary conditions [1], does also apply for the present case.

For a general potential V(x), (2) and (8) present the following type of solutions

$$\Psi(x,t) = \exp\left(-\frac{iE_{\psi}t}{\hbar}\right)\psi(x) , \qquad (17)$$

$$\Phi(x,t) = \exp\left(\frac{iE_{\phi}t}{\hbar}\right)\phi(x), \qquad (18)$$

leading to the set of time-independent equations

$$E_{\psi}\psi = -\frac{\hbar^2}{2m} \left(1 + \gamma x^2\right)^2 \frac{d^2\psi}{dx^2} - \frac{\hbar^2\gamma}{m} x \left(1 + \gamma x^2\right) \frac{d\psi}{dx} + V(x)\psi , \qquad (19)$$

$$E_{\phi}\phi = -\frac{\hbar^2}{2m} \left( 1 + \gamma x^2 \right)^2 \frac{d^2\phi}{dx^2} - \frac{3\hbar^2\gamma}{m} x \left( 1 + \gamma x^2 \right) \frac{d\phi}{dx}$$
$$- \frac{\hbar^2\gamma}{m} \left( 1 + 3\gamma x^2 \right) \phi + V(x)\phi . \tag{20}$$

The solution proposed in (17) and (18) is very general, with  $E_{\psi}=(E_{\phi})^*$ . However, the PT symmetry should lead to a real energy spectrum, i.e.,  $E_{\psi}=E_{\phi}=E$ , yielding in (10) a time-independent probability density at the



stationary state. Hence, one has the pair of time-independent equations

$$E\psi(x) = \hat{H}\psi(x) ; \qquad E\phi(x) = \hat{H}^{\dagger}\phi(x) , \qquad (21)$$

where the operators  $\hat{H}$  and  $\hat{H}^{\dagger}$  are defined in (19) and (20), respectively. Now, at the stationary state, a somewhat lengthy (but straightfoward) calculation by considering a sequence of two integrations by parts and assuming the conditions that  $\psi(x)$ ,  $\phi(x)$ ,  $(d\psi(x)/dx)$ , and  $(d\phi(x)/dx)$  should go to zero faster than  $x^{-2}$ , in the limit  $|x| \to \infty$ , than one can find  $\hat{H}^{\dagger}$  of (20) from the operator  $\hat{H}$  of (19) in the usual way [1],

$$\int_{-\infty}^{\infty} dx \, \phi(x) \hat{H} \psi(x) = \int_{-\infty}^{\infty} dx \, \psi(x) \hat{H}^{\dagger} \phi(x) . \qquad (22)$$

The equation above confirms that  $\phi(x)$  corresponds to the left eigenstate of the operator  $\hat{H}$ , or to the right eigenstate of  $\hat{H}^{\dagger}$ ; moreover, considering the present solutions, (15) and (16) yield  $\langle \hat{H} \rangle = \langle \hat{H}^{\dagger} \rangle = E$ .

In the next section, we will work with (19) and (20) for some standard choices of the potential V(x).

### 3 Simple Applications

# 3.1 Particle in a Constant Potential

As a first example, let us consider a constant potential,  $V(x) = V_0 \ge 0 \ (-\infty < x < \infty)$ . Hence, one has a pair of solutions

$$\psi(x) = C_1 \exp\left[\frac{ik}{\sqrt{\gamma}}\arctan(\sqrt{\gamma}x)\right],$$
 (23)

$$\phi(x) = \frac{C_2}{1 + \gamma x^2} \exp\left[\frac{-ik}{\sqrt{\gamma}} \arctan(\sqrt{\gamma}x)\right], \qquad (24)$$

where  $k = [2m(E - V_0)]^{1/2}/\hbar$ . The case  $V_0 = 0$ , to be called herein as the "free-particle solution", comes naturally from the above equations, as expected, and will be discussed below. One remarkable aspect of these solutions corresponds to the finiteness of the integral of the probability density defined in (10) for  $\gamma > 0$ 

$$\int_{-\infty}^{\infty} dx \, \rho(x) = \int_{-\infty}^{\infty} dx \, \frac{C_1 C_2 + C_1^* C_2^*}{2(1 + \gamma x^2)}$$
$$= \frac{\pi}{2\sqrt{\gamma}} \left( C_1 C_2 + C_1^* C_2^* \right) , \tag{25}$$

from which one considers  $C_1C_2 + C_1^*C_2^* = 2\sqrt{\gamma}/\pi$  for normalization. From now on, we will restrict ourselves to real coefficients, so that  $C_2 = \sqrt{\gamma}/(\pi C_1)$ , leading to a

Lorentzian probability density

$$\rho(x) = \frac{\sqrt{\gamma}}{\pi (1 + \gamma x^2)} \,. \tag{26}$$

Therefore, within the present proposal, one does not need to confine the particle in a box for normalizability; as expected, the usual nonintegrability of the free-particle solution with a constant mass,  $m_e(x) = m$ , is recovered in full space  $(-\infty < x < \infty)$  in the limit  $\gamma \to 0$ . For  $\gamma > 0$ , the solutions of (23) and (24) represent a localized particle around the origin, since  $\langle x \rangle = \int_{-\infty}^{\infty} dx \, x \rho(x) = 0$ .

The next important point concerns the quantization of the energy spectrum; we will show below that this property comes directly from the orthogonality of these solutions. For that, we consider (23) and (24) with wave vectors k and k', to be denoted by  $\psi_k(x)$  and  $\phi_{k'}(x)$  respectively, such as to define the integral,

$$\mathcal{I}_{k,k'} = \int_{-\infty}^{\infty} dx \, \psi_k(x) \phi_{k'}(x)$$

$$= \frac{\sqrt{\gamma}}{\pi} \int_{-\infty}^{\infty} \frac{dx}{1 + \gamma x^2} \exp\left[\frac{i(k - k')}{\sqrt{\gamma}} \arctan(\sqrt{\gamma}x)\right]$$
(27)

Introducing the variable  $y = (1/\sqrt{\gamma})\arctan(\sqrt{\gamma}x)$ , the integral above becomes

$$\mathcal{I}_{k,k'} = \frac{\sqrt{\gamma}}{\pi} \int_{-\pi/(2\sqrt{\gamma})}^{\pi/(2\sqrt{\gamma})} dy \, \exp\left[i(k-k')y\right]$$
$$= \frac{\sqrt{\gamma}}{\pi} \frac{2}{k-k'} \sin\left[\frac{(k-k')\pi}{2\sqrt{\gamma}}\right]. \tag{28}$$

Since the imaginary part of the integral defined in (27) does not contribute, the inner product defined in (13) is precisely this integral

$$(\psi_{k}(x), \phi_{k'}(x)) = \frac{1}{2} \int_{-\infty}^{\infty} dx \left[ \psi_{k}(x)\phi_{k'}(x) + \psi_{k}^{*}(x)\phi_{k'}^{*}(x) \right]$$

$$= \frac{\sqrt{\gamma}}{\pi} \int_{-\infty}^{\infty} \frac{dx}{1 + \gamma x^{2}} \cos \left[ \frac{(k - k')}{\sqrt{\gamma}} \arctan(\sqrt{\gamma}x) \right]$$

$$= \mathcal{I}_{k,k'}. \tag{29}$$

An important property of the eigenfunctions of an Hermitian operator is their orthogonality [1]. This property can be shown by considering the integral

$$\int_{-\infty}^{\infty} dx \phi_{k'}(x) \hat{H} \psi_k(x) = E_k \int_{-\infty}^{\infty} dx \phi_{k'}(x) \psi_k(x) , \qquad (30)$$

which becomes, after an integration by parts,

$$\int_{-\infty}^{\infty} dx \, \hat{H}^{\dagger} \phi_{k'}(x) \psi_k(x) = E_{k'} \int_{-\infty}^{\infty} dx \phi_{k'}(x) \psi_k(x) . \tag{31}$$

Since these two integrals are equal, one has that

$$(E_k - E_{k'}) \int_{-\infty}^{\infty} dx \, \psi_k(x) \phi_{k'}(x) = (E_k - E_{k'}) \mathcal{I}_{k,k'} = 0, \quad (32)$$



with a similar result applying to the corresponding complexconjugate eigenstates. Since the eigenstates  $\phi_k(x)$  and  $\psi_k(x)$  are normalized, one has the orthogonality condition,  $\mathcal{I}_{k,k'} = \delta_{k,k'}$ , and consequently

$$(\psi_k(x), \phi_{k'}(x)) = \delta_{k,k'}. \tag{33}$$

By considering this, one is left with a discretization for the wave vectors

$$k - k' = 2j\sqrt{\gamma}$$
  $(j = 0, \pm 1, \pm 2, \cdots)$ , (34)

where one notices the case j=0, i.e., k=k', corresponding to the normalization condition considered in (25).

Hence, in order to satisfy (34), one notices that the free particle should present a discrete energy spectrum,  $E_n = \hbar^2 k_n^2/(2m)$ , where the set of wave vectors  $\{k_n\}$  may be taken from either one of the following series

Even series: 
$$k_n = 2n\sqrt{\gamma}$$
, (35)

Odd series: 
$$k_n = (2n+1)\sqrt{\gamma}$$
, (36)

with  $n=0,\pm 1,\pm 2,\cdots$ . From both series above, one sees that the quantum of momentum is  $\delta p=\hbar(k_{n+1}-k_n)=2\hbar\sqrt{\gamma}$ , leading to a physical interpretation for the deformation parameter  $\gamma$ . One should stress that  $\delta p\to 0$ , when  $\gamma\to 0$ , i.e., the continuous spectrum of the free-particle within the standard SE is recovered. The energy spectra corresponding to these two types of solutions are

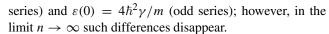
$$E_n = \frac{\hbar^2 k_n^2}{2m} = \begin{cases} 2\hbar^2 n^2 \gamma/m, & \text{even series }, \\ \hbar^2 (2n+1)^2 \gamma/2m, & \text{odd series }, \end{cases}$$
(37)

where one sees that in the later series the zero of energy is shifted by a constant,  $E_0 = \hbar^2 \gamma/2m$ . The quantum of energy depends on n,  $\varepsilon(n) = E_{n+1} - E_n$ , being given by

$$\varepsilon(n) = \frac{\hbar^2}{2m} \left( k_{n+1}^2 - k_n^2 \right)$$

$$= \begin{cases} 2\hbar^2 (2n+1)\gamma/m , & \text{even series }, \\ 4\hbar^2 (n+1)\gamma/m , & \text{odd series }. \end{cases}$$
(38)

One notices that  $\varepsilon(n)$  presents significant differences from one series to the other for low values of n, e.g., the gap  $\varepsilon(0) = E_1 - E_0$  is given by  $\varepsilon(0) = 2\hbar^2 \gamma/m$  (even



As usual, the pair of solutions in (23) and (24) may be written also in the form

$$\psi_k(x) = a_1 \cos\left[\alpha_k(x)\right] + a_2 \sin\left[\alpha_k(x)\right] , \qquad (39)$$

$$\phi(x) = \frac{1}{1 + \nu x^2} \{ b_1 \cos \left[ \alpha_k(x) \right] + b_2 \sin \left[ \alpha_k(x) \right] \}, \quad (40)$$

$$\alpha_k(x) = \frac{k}{\sqrt{\gamma}} \arctan(\sqrt{\gamma}x)$$
, (41)

which may be more appropriate when dealing with boundary-condition problems, like in the next application.

### 3.2 Particle in an Infinite Square Well Potential

As a second illustration, we consider a particle described by (19) and (20) under the potential of an infinite square well, i.e., infinite for x < -L and x > L, and zero in the interval -L < x < L. Like the standard SE [1], we impose the wave functions  $\psi(x)$  and  $\phi(x)$  to be zero when the potential is infinite,  $\psi(-L) = \psi(L) = \phi(-L) = \phi(L) = 0$ . Considering the simplest case where  $E_{\psi} = E_{\phi} = E$ , possible solutions of the form presented in (39) and (40) are

$$\psi_n(x) = A_n \sin\left[\frac{k_n}{\sqrt{\gamma}}\arctan(\sqrt{\gamma}x)\right],$$
 (42)

$$\phi_n(x) = \frac{A_n}{(1 + \gamma x^2)} \sin \left[ \frac{k_n}{\sqrt{\gamma}} \arctan(\sqrt{\gamma} x) \right], \qquad (43)$$

if -L < x < L, and  $\psi_n(x) = \phi_n(x) = 0$ , otherwise. Imposing the boundary conditions above, the wave vectors become quantized

$$k_n = \frac{n\pi\sqrt{\gamma}}{\arctan(\sqrt{\gamma}L)}; \qquad (n = 0, \pm 1, \pm 2, \cdots), \qquad (44)$$

leading to the following energy eigenvalues

$$E_n = \frac{\hbar^2 n^2 \pi^2 \gamma}{2m \arctan^2(\sqrt{\gamma}L)}; \qquad (n = 0, \pm 1, \pm 2, \cdots).$$
 (45)

The coefficient  $A_n$  that appears in (42) and (43) is a normalization factor and is computed by imposing  $\int_{-L}^{L} dx \rho(x) = 1$ . In this case, one uses the probability density of (10) to obtain

$$A_n^2 = \frac{\sqrt{\gamma}}{\arctan(\sqrt{\gamma}L)} \,. \tag{46}$$

One should notice that in the limit  $\gamma \to 0$  one gets  $A_n^2 = 1/L$ , which diverges in the limit  $L \to \infty$ , as



expected. However, for  $\gamma > 0$ , the normalization factor is always finite, and particularly in the limit  $L \to \infty$  one gets  $A_n^2 = 2\sqrt{\gamma}/\pi$ . This result is in agreement with the previous analysis of the free particle in open space [cf. (25)], where one identifies  $A_n^2 = 2C_1C_2 = 2\sqrt{\gamma}/\pi$ , as one goes from the plane-wave forms of (23) and (24) to those in (39) and (40). Moreover, in limit  $L \to \infty$ , one verifies that the discretization of wave vectors of (44) recovers the even series of (35). In the present case, the above quantization of wave vectors leads naturally to the orthogonality of the solutions, i.e.,  $(\psi_n, \phi_{n'}) = \delta_{n,n'}$ .

We will now discuss a second pair of solutions for the infinite square well, which in the limit  $L \to \infty$  should yield the odd series of (36). One sees that an equivalent pair of solutions in this case is obtained by replacing  $\sin[..] \to \cos[..]$  in (42) and (43). For this solution to satisfy the boundary conditions, one should have

$$k_n = \frac{(n+1/2)\pi\sqrt{\gamma}}{\arctan(\sqrt{\gamma}L)}; \qquad (n=0,\pm 1,\pm 2,\cdots),$$
 (47)

leading to the following energy eigenvalues

$$E_n = \frac{\hbar^2 (n + 1/2)^2 \pi^2 \gamma}{2m \arctan^2(\sqrt{\gamma} L)}; \qquad (n = 0, \pm 1, \pm 2, \cdots).$$
(48)

This second pair of solutions corresponds precisely to the odd series of (36), in the limit  $L \to \infty$ .

It is important to stress the two different procedures used herein to obtain the quantization of wave vectors: (i) Imposing the orthogonality of solutions, as done for the free-particle in full space  $(-\infty < x < \infty)$ ; (ii) Considering appropriate boundary conditions for a particle in an infinite square well (-L < x < L). These two procedures were shown to be equivalent in the limit  $L \to \infty$ .

### 4 Three-Dimensional Case

Herein, we will generalize the previous results to three dimensions; in this case, (2) becomes

$$i\hbar \frac{\partial \Psi(\vec{x},t)}{\partial t} = \hat{H}\Psi(\vec{x},t)$$

$$= -\frac{\hbar^2}{2}\hat{D}_m^2\Psi(\vec{x},t) - \frac{\hbar^2}{4}\left[\vec{\nabla}\left(\frac{1}{m_e}\right)\right] \cdot \vec{\nabla}\Psi(\vec{x},t)$$

$$+ V(\vec{x})\Psi(\vec{x},t), \qquad (49)$$

which defines the Hamiltonian

$$\hat{H} = -\frac{\hbar^2}{2}\hat{D}_m^2 - \frac{\hbar^2}{4} \left[ \vec{\nabla} \left( \frac{1}{m_e} \right) \right] \cdot \vec{\nabla} + V(\vec{x}) . \tag{50}$$

In the equations above  $\vec{x} \equiv (x_1, x_2, x_3)$  and we consider

$$\hat{D}_{m}^{2} \equiv \frac{1}{m_{e_{1}}} \frac{\partial^{2}}{\partial x_{1}^{2}} + \frac{1}{m_{e_{3}}} \frac{\partial^{2}}{\partial x_{2}^{2}} + \frac{1}{m_{e_{3}}} \frac{\partial^{2}}{\partial x_{3}^{2}},$$
 (51)

$$\vec{\nabla} \left( \frac{1}{m_e} \right) \equiv \left[ \frac{\partial}{\partial x_1} \left( \frac{1}{m_{e_1}} \right), \frac{\partial}{\partial x_2} \left( \frac{1}{m_{e_2}} \right), \frac{\partial}{\partial x_3} \left( \frac{1}{m_{e_3}} \right) \right], \quad (52)$$

$$\vec{\nabla}^2 \left( \frac{1}{m_e} \right) \equiv \left[ \frac{\partial^2}{\partial x_1^2} \left( \frac{1}{m_{e_1}} \right), \frac{\partial^2}{\partial x_2^2} \left( \frac{1}{m_{e_2}} \right), \frac{\partial^2}{\partial x_3^2} \left( \frac{1}{m_{e_3}} \right) \right], (53)$$

with  $m_{e_i}(x_i) = m/(1 + \gamma x_i^2)^2$  for i = 1, 2, 3. The proposal above corresponds to a very general type of particle's position-dependent effective mass, following parity symmetry  $[m_{e_i}(-x_i) = m_{e_i}(x_i)]$  and characterized by a spatial anisotropy. Moreover, one should have as well  $V(-\vec{x}) = V(\vec{x})$ .

The classical field theory introduced above for the onedimensional case may be extended to three dimensions. In this case, the Euler-Lagrange equation for the field  $\Phi(\vec{x}, t)$ yields (49), whereas the one for the field  $\Psi(\vec{x}, t)$  leads to the equation for the extra field  $\Phi(\vec{x}, t)$ , namely,

$$-i\hbar \frac{\partial \Phi(\vec{x}, t)}{\partial t} = \hat{H}^{\dagger} \Phi(\vec{x}, t)$$

$$= -\frac{\hbar^2}{2} \hat{D}_m^2 \Phi(\vec{x}, t) - \frac{3\hbar^2}{4} \left[ \vec{\nabla} \left( \frac{1}{m_e} \right) \right] \cdot \vec{\nabla} \Phi(\vec{x}, t)$$

$$- \frac{\hbar^2}{4} \left[ \vec{\nabla}^2 \left( \frac{1}{m_e} \right) \right] \Phi(\vec{x}, t) + V(\vec{x}) \Phi(\vec{x}, t) , \quad (54)$$

corresponding to

$$\hat{H}^{\dagger} = -\frac{\hbar^2}{2} \, \hat{D}_m^2 - \frac{3\hbar^2}{4} \left[ \vec{\nabla} \left( \frac{1}{m_e} \right) \right] \cdot \vec{\nabla} - \frac{\hbar^2}{4} \left[ \vec{\nabla}^2 \left( \frac{1}{m_e} \right) \right] + V(\vec{x}) \,. \tag{55}$$

Considering the fields  $\Psi(\vec{x}, t)$  and  $\Phi(\vec{x}, t)$  above, one defines the probability density

$$\rho(\vec{x},t) = \frac{1}{2} \left[ \Psi(\vec{x},t) \Phi(\vec{x},t) + \Psi^*(\vec{x},t) \Phi^*(\vec{x},t) \right], \quad (56)$$

which follows a continuity equation in three dimensions

$$\frac{\partial \rho(\vec{x},t)}{\partial t} + \vec{\nabla} \cdot \vec{j}(\vec{x},t) = 0, \qquad (57)$$

where the current-density vector  $\vec{j}(\vec{x}, t)$  is given by a three-dimensional generalization of the form in (12). Like in the one-dimensional case, the above continuity equation applies for general  $m_e(\vec{x})$  and  $V(\vec{x})$ , ensuring the conservation of probability for all times.



By writing (49) and (54) in terms of Cartesian components, one obtains

$$i\hbar \frac{\partial \Psi(\vec{x}, t)}{\partial t} = -\frac{\hbar^2}{2m} \sum_{i=1,2,3} \left[ (1 + \gamma x_i^2)^2 \frac{\partial^2 \Psi(\vec{x}, t)}{\partial x_i^2} \right]$$
$$-\frac{\hbar^2 \gamma}{m} \sum_{i=1,2,3} \left[ x_i (1 + \gamma x_i^2) \frac{\partial \Psi(\vec{x}, t)}{\partial x_i} \right]$$
$$+V(\vec{x})\Psi(\vec{x}, t) , \qquad (58)$$

$$i\hbar \frac{\partial \Phi(\vec{x}, t)}{\partial t} = -\frac{\hbar^2}{2m} \sum_{i=1,2,3} \left[ \left( 1 + \gamma x_i^2 \right)^2 \frac{\partial^2 \Phi(\vec{x}, t)}{\partial x_i^2} \right]$$
$$-\frac{3\hbar^2 \gamma}{m} \sum_{i=1,2,3} \left[ x_i \left( 1 + \gamma x_i^2 \right) \frac{\partial \Phi(\vec{x}, t)}{\partial x_i} \right]$$
$$-\frac{\hbar^2 \gamma}{m} \sum_{i=1,2,3} \left[ \left( 1 + 3\gamma x_i^2 \right) \Phi(\vec{x}, t) \right]$$
$$+V(\vec{x}) \Phi(\vec{x}, t) . \tag{59}$$

Solutions similar to those of (17) and (18) hold herein also,

$$\Psi(\vec{x},t) = \exp\left(-\frac{iEt}{\hbar}\right)\psi(\vec{x}), \qquad (60)$$

$$\Phi(\vec{x},t) = \exp\left(\frac{iEt}{\hbar}\right)\phi(\vec{x}), \qquad (61)$$

where for the present case, one has

$$\psi(\vec{x}) = \psi_1(x_1)\psi_2(x_2)\psi_3(x_3); \quad \phi(\vec{x}) = \phi_1(x_1)\phi_2(x_2)\phi_3(x_3).$$
 (62)

Substituting these solutions into (58) and (59) one obtains, respectively,

$$-\frac{\hbar^2}{2m} \sum_{i=1,2,3} \left[ \left( 1 + \gamma x_i^2 \right)^2 \frac{1}{\psi_i(x_i)} \frac{\partial^2 \psi_i(x_i)}{\partial x_i^2} \right]$$

$$-\frac{\hbar^2 \gamma}{m} \sum_{i=1,2,3} \left[ x_i \left( 1 + \gamma x_i^2 \right) \frac{1}{\psi_i(x_i)} \frac{\partial \psi_i(x_i)}{\partial x_i} \right]$$

$$= E - V(\vec{x}), \qquad (63)$$

$$-\frac{\hbar^2}{2m} \sum_{i=1,2,3} \left[ \left( 1 + \gamma x_i^2 \right)^2 \frac{1}{\phi_i(x_i)} \frac{\partial^2 \phi_i(x_i)}{\partial x_i^2} \right]$$

$$-\frac{3\hbar^2 \gamma}{m} \sum_{i=1,2,3} \left[ x_i \left( 1 + \gamma x_i^2 \right) \frac{1}{\phi_i(x_i)} \frac{\partial \phi_i(x_i)}{\partial x_i} \right]$$

$$-\frac{\hbar^2 \gamma}{m} \sum_{i=1,2,3} \left( 1 + 3\gamma x_i^2 \right) = E - V(\vec{x}) . \tag{64}$$

From now on, we restrict ourselves to a constant potential,  $V(\vec{x}) = V_0 \ge 0$ . Hence, one has the following pair of

solutions for each Cartesian component i,

$$\psi_i(x_i) = C_{1i} \exp\left[\frac{ik_i}{\sqrt{\gamma}}\arctan(\sqrt{\gamma}x_i)\right],$$
 (65)

$$\phi_i(x_i) = \frac{C_{2i}}{1 + \gamma x_i^2} \exp\left[\frac{-ik_i}{\sqrt{\gamma}}\arctan(\sqrt{\gamma}x_i)\right], \qquad (66)$$

with  $E - V_0 = (\hbar^2/2m) (k_1^2 + k_2^2 + k_3^2)$ . Next, we discuss the simple case of a free particle.

#### 4.1 Free Particle

Like in the one-dimensional case, a free particle will be considered as the particular limit  $V_0 = 0$ ; the solutions above lead to

$$\Psi(\vec{x}, t) = a \exp\left(-\frac{iEt}{\hbar}\right) \exp\left[i\alpha(\vec{x})\right] , \qquad (67)$$

$$\Phi(\vec{x}, t) = \frac{b}{(1 + \gamma x_1^2)(1 + \gamma x_2^2)(1 + \gamma x_2^2)} \exp\left(\frac{iEt}{\hbar}\right) \exp\left[-i\alpha(\vec{x})\right] (68)$$

$$\alpha(\vec{x}) = \sum_{i=1,2,3} \frac{k_i}{\sqrt{\gamma}} \arctan(\sqrt{\gamma} x_i) , \qquad (69)$$

with 
$$E = (\hbar^2/2m)(k_1^2 + k_2^2 + k_3^2)$$
.

Like before, within the present proposal, one has a freeparticle solution characterized by a finite norm,

$$\int d\vec{x} \; \rho(\vec{x}, t) = \frac{1}{2} \int d\vec{x} \; \left[ \Psi(\vec{x}, t) \Phi(\vec{x}, t) + \Psi^*(\vec{x}, t) \Phi^*(\vec{x}, t) \right]$$

$$= ab \left[ \int_{-\infty}^{\infty} dx_1 \frac{1}{(1 + \gamma x_1^2)} \right]$$

$$\times \left[ \int_{-\infty}^{\infty} dx_2 \frac{1}{(1 + \gamma x_2^2)} \right] \left[ \int_{-\infty}^{\infty} dx_3 \frac{1}{(1 + \gamma x_3^2)} \right]$$

$$= \frac{ab, \pi^3}{\gamma^{3/2}} \; , \tag{70}$$

which requires  $ab = \gamma^{3/2}/\pi^3$  for normalization. Consequently, this solution represents a particle localized around the origin (since  $\langle x_i \rangle = 0$  for each component), with the probability density  $\rho(\vec{x},t)$  presenting two important ingredients: (i) A finite norm; (ii) It follows a continuity equation [cf. (57)] for all times. Considering the solutions in (67)–(69), one has

$$\rho(\vec{x},t) = \rho(\vec{x}) = \frac{\gamma^{3/2}}{\pi^3} \frac{1}{\left(1 + \gamma x_1^2\right) \left(1 + \gamma x_2^2\right) \left(1 + \gamma x_3^2\right)}, \quad (71)$$

representing the three-dimensional extension of (26). As expected, in the limit  $\gamma \to 0$ , one recovers the constant-mass free-particle solution with  $m_e(\vec{x}) = m$  and  $\rho(\vec{x}) =$  constant, characterizing a nonintegrability in full space.



Similarly to the one-dimensional case, the quantization comes by imposing orthogonality of the solutions above [cf. (27)]

$$\mathcal{I}_{\vec{k},\vec{k}'} = \int d\vec{x} \psi_{\vec{k}}(\vec{x}) \,\phi_{\vec{k}}(\vec{x}) = \frac{\gamma^{3/2}}{\pi^3} \left[ \int_{-\infty}^{\infty} dx_1 \, \frac{1}{(1+\gamma x_1^2)} \exp\left\{i \frac{k_1 - k_1'}{\sqrt{\gamma}} \arctan(\sqrt{\gamma} x_1)\right\} \right] \\
\times \left[ \int_{-\infty}^{\infty} dx_2 \, \frac{1}{(1+\gamma x_2^2)} \exp\left\{i \frac{k_2 - k_2'}{\sqrt{\gamma}} \arctan(\sqrt{\gamma} x_2)\right\} \right] \\
\times \left[ \int_{-\infty}^{\infty} dx_3 \, \frac{1}{(1+\gamma x_3^2)} \exp\left\{i \frac{k_3 - k_3'}{\sqrt{\gamma}} \arctan(\sqrt{\gamma} x_3)\right\} \right], \tag{72}$$

leading to two set of quantized wave vectors for each Cartesian component, namely [cf. (35)],

Even series: 
$$k_{n_i} = 2n_i \sqrt{\gamma}$$
, (73)

Odd series: 
$$k_{n_i} = (2n_i + 1)\sqrt{\gamma}$$
, (74)

with  $n_i=0,\pm 1,\pm 2,\cdots$  (i=1,2,3). The quantum of momentum in each component is given by  $\delta p_i=\hbar(k_{n_i+1}-k_{n_i})=2\hbar\sqrt{\gamma}$ , showing that the deformation parameter  $\gamma$  is directly related to the quantization, i.e.,  $\delta p_i\to 0$ , when  $\gamma\to 0$ .

Hence, we have shown in the present section that the anisotropy introduced herein in the effective mass, characterized by independence in the Cartesian directions,  $m_{e_i}(x_i) = m/\left(1 + \gamma x_i^2\right)^2$  for i = 1, 2, 3, allows to extend the one-dimensional results of the previous sections to three-dimensions. From the results above, the formulation of the problem for an arbitrary number of dimensions becomes straightforward.

#### **5** Conclusions

To conclude, we have introduced a non-Hermitian PT symmetric Hamiltonian  $\hat{H}$ , characterized by position-dependent masses, from which a linear Schrödinger equation,  $i\hbar$ ,  $[\partial\Psi(x,t)/\partial t] = \hat{H}\Psi(x,t)$ , was defined. This equation emerged through a deformed differential operator, characterized by a positive deformation parameter  $\gamma$ . Such a deformation is very similar to those used frequently on nonextensive statistical mechanics, such that the standard differential operator is recovered when  $\gamma \to 0$ . Within the present proposal, one has  $\hat{H}^\dagger \neq \hat{H}$  for  $\gamma > 0$ , whereas Hermiticity is recovered only in the limit  $\gamma \to 0$ . Previous approaches, based on an exact classical field theory, have shown the necessity of an extra field  $\Phi(x,t)$  for

these classes of equations, where the field  $\Phi(x, t)$  becomes  $\Psi^*(x, t)$  only when  $\hat{H}^{\dagger} = \hat{H}$ , i.e.,  $\gamma = 0$ . This extra field satisfies the conjugate equation,  $-i\hbar$ ,  $[\partial \Phi(x, t)/\partial t] = \hat{H}^{\dagger}\Phi(x, t)$ .

Considering an appropriate probability density, defined in terms of both fields  $\Psi(x,t)$  and  $\Phi(x,t)$ , a continuity equation follows, guaranteeing the preservation of probability. The introduction of the extra field  $\Phi(x,t)$  is mandatory for a continuity equation, and consequently, for a consistent definition of a probability density that is conserved. For this class of mass-dependent Schrödinger equations, this result is not possible (as far as we know) by considering only the Schrödinger equation and its complex conjugate; however, by introducing the extra field  $\Phi(x,t)$ , following the corresponding conjugate equation, the continuity equation follows for a general effective mass  $m_e(x)$  and external potential V(x). It is also shown that the new field  $\Phi(x,t)$  corresponds to the left eigenstate of the operator  $\hat{H}$ , or to the right eigenstate of  $\hat{H}^{\dagger}$ .

The equations for the two fields were solved analytically in simple cases, namely, a free particle in full space, and a particle in an infinite square well (-L < x < L). For the free particle, the quantization of momenta was obtained by imposing the orthogonality of solutions, yielding a quantum of momentum  $\delta p = \hbar (k_{n+1} - k_n) = 2\hbar \sqrt{\gamma}$ , providing a physical interpretation for the deformation parameter  $\gamma$ within the present approach. For the particle in the square well the standard procedure was considered, i.e., imposing boundary conditions. These two schemes for quantization were shown to be equivalent in the limit  $L \to \infty$ . The freeparticle solution studied herein has exhibited the remarkable property of integrability in full space, being characterized by a finite norm. This result is to be contrasted with the freeparticle within the standard Schrödinger equation, for which the plane-wave solution does not present a well-defined norm.

A three-dimensional proposal was also presented, in terms of the two fields  $\Psi(\vec{x}, t)$  and  $\Phi(\vec{x}, t)$ , being characterized by an anisotropic form for the



position-dependent masses. It was shown that all results obtained in the one-dimensional analysis should hold for each Cartesian component independently. Particularly, the quantization and normalizability of the free-particle solution in full open space were demonstrated, identifying a particle localized around the origin. Hence, analogously to what happens in the standard Schrödinger equation, the wave packet procedure, where a localized wave is obtained by a superposition of plane waves, may be also used herein; however, as we have shown above, a localized wave appears naturally through the solutions of the nonlinear equations associated to the fields  $\Psi(\vec{x},t)$  and  $\Phi(\vec{x},t)$ .

For the purposes of the present work, physical systems characterized by interfaces where changes in the chemical composition exist should be relevant. Particularly, good candidates are semiconductor heterostructures, which are composed by sets of such interfaces (i.e., heterojunctions) and are well known to produce position-dependent effective masses. In these heterojunctions, the chemical changes do not occur abruptly, but instead, they are graded over some specified distance, and consequently, the effective mass should be a continuous function of the position. Hence, for an electron moving inside such a structure, its mass varies continuously with the position, and so it should be describable by a mass-dependent Schrödinger equation. The present proposal for effective mass,  $m_e(x) =$  $m/(1+\gamma x^2)^2$ , leads to a maximum probability density at the origin, decreasing continuously for increasing values of |x|, and represents typically the physical situation that occurs with the concentration of electrons in pnp junctions. The parameter  $\gamma$  should be adjusted from measurements and is expected to depend on the particular types of materials used in the junctions.

**Acknowledgments** We thank C. Tsallis for fruitful conversations. The partial financial supports from CNPq and FAPERJ (Brazilian agencies) are acknowledged.

#### References

- R.L. Liboff, Introductory Quantum Mehanics, 4th edn. (Addison Wesley, San Francisco, 2003)
- C. Sulem, P.-L. Sulem, The Nonlinear Schrödinger Equation: Self-Focusing and Wave Collapse (Springer, New York, 1999)
- 3. A.C. Scott, *The nonlinear universe* (Springer, Berlin, 2007)
- 4. F.D. Nobre, M.A. Rego-Monteiro, C. Tsallis, Phys. Rev. Lett. 106 (2011)
- F.D. Nobre, M.A. Rego-Monteiro, C. Tsallis, Europhys. Lett. 97, 41001 (2012)
- 6. A.R. Plastino, C. Tsallis, J. Math. Phys. 54, 041505 (2013)
- M.A. Rego-Monteiro, F.D. Nobre, J. Math. Phys. 54, 103302 (2013)
- 8. C. Tsallis, Introduction to nonextensive statistical mechanics (Springer, New York, 2009)
- 9. O. von Roos, Phys. Rev. B 27, 7547 (1983)
- 10. J.-M. Lévy-Leblond, Phys. Rev. A 52, 1845 (1995)
- A.R. Plastino, A. Rigo, M. Casas, F. Garcias, A. Plastino, Phys. Rev. A 60, 4318 (1999)
- 12. S.-H. Dong, M. Lozada-Cassou, Phys. Lett. A 337, 313 (2005)
- 13. C. Quesne, J. Phys. A 40, 13107 (2007)
- R.N. Costa Filho, M.P. Almeida, G.A. Farias, J.S.Jr. Andrade, Phys. Rev. A 84, 050102(R) (2011)
- 15. S.H. Mazharimousavi, Phys. Rev. A 85, 034102 (2012)
- R.N. Costa Filho, G. Alencar, B.-S. Skagerstam, J.S. Andrade Jr., Europhys. Lett. 101, 10009 (2013)
- 17. M.A. Rego-Monteiro, F.D. Nobre, Phys. Rev. A 88, 032105 (2013)
- 18. G. Bastard, Wave mechanics applied to semiconductor heterostructures (Les Editions de Physique Les Ulis, France, 1988)
- C. Weisbuch, B. Vinter, Quantum semiconductor structures: Fundamentals and applications (Academic Press, New York, 1991)
- 20. C.M. Bender, Rep. Prog. Phys. **70**, 947 (2007)
- F.G. Scholtz, H.B. Geyer, F.J.W. Hahne, Ann. Phys. 213, 74 (1992)
- 22. C.M. Bender, S. Boettcher, Phys. Rev. Lett. 80, 5243 (1998)
- 23. F. Cannata, G. Junker, J. Trost, Phys. Lett. A 246, 219 (1998)
- C.M. Bender, D.C. Brody, H.F. Jones, Phys. Rev. Lett. 89, 270401 (2002)
- 25. A. Mostafazadeh, J. Math. Phys. 43, 2814 (2002)
- J. da Providência, N. Bebiano, J.P. da Providência, Braz. J. Phys. 41, 78 (2011)
- 27. S. Dey, A. Fring, Phys. Rev. D 86, 064038 (2012)
- 28. E.P. Borges, Physica A 340, 95 (2004)
- 29. C.G. Bollini, J.J. Giambiagi, Braz. J. Phys. 17, 14 (1987)
- 30. J. Barcelos-Neto, N.R.F. Braga, Acta Phys. Pol. B 20, 205 (1989)

