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Non-additive quantum mechanics for a position-dependent mass system: Dirac delta and quasi-periodic potentials

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Abstract – Motivated by non-extensive statistical mechanics, in this work we consider a deformed Schrödinger equation (DSE) for position-dependent mass (PDM) systems, whose deformed plane-wave solutions allow to characterise a non-periodic lattice. We obtain a deformed version of the Bloch theorem and we illustrate the formalism presented with two examples of the literature: the Dirac and the Kronig-Penney potentials. We found that the Kronig-Penney potential offers a modelling for a lattice with defects expressed by a non-periodicity of the potential within the underlying non-extensive mathematical structure, which is evidenced by the displacement of the gaps with respect to the non-deformed case. The eigenfunctions, the reduced energy bands scheme and the density of states are affected by the deformation.

Introduction. – Quantum mechanics is one of most robust theories of modern physics. Its wide applicability in multiple phenomena is reflected in the actual advances in science and technology. In particular, quantum mechanics allows to explain the transport phenomena of particles in solid mediums. In this field, a remarkable contribution was made by Felix Bloch [1] by studying the transport of electrons in periodic potentials from the Schrödinger equation, whose result is the well-known Bloch theorem. This theorem expresses that the wave function of the conduction electrons in a perfect crystal (*i.e.*, when the potential has a discrete symmetry in the position coordinates) is a Bloch wave function satisfying the same symmetry of the potential. However, in real systems the presence of defects, impurities, thermal vibrations and other effects in the crystal lattice makes the Bloch theorem insufficient to describe these features. In this scenario and also in more complex structures, news formulations of the Bloch theorem turn out to be necessary. One possibility is to consider a position-dependent mass (PDM) (*i.e.*, a mass continuously distributed in the space as $m(\hat{x})$), that suggests the use of a generalised Schrödinger equation (or Hamiltonian) associated with an appropriate deformed kinetic term to model characteristics of real solids.

Hamiltonians with a PDM have been investigated in many areas of the physics, both experimentally and theoretically: semiconductors [2], quantum dots [3], many body theory [4], super-symmetrical quantum mechanics [5], quantum liquids [6], inversion potential for NH_3 [7], astrophysics [8], non-linear optics [9], relativistic quantum mechanics [10], classical field theory [11], nuclear physics [12], etc. Usually, in quantum systems with a PDM, the mass function $m(\hat{x})$ and the linear momentum are non-commutating operators. A detailed analysis has been performed using the mathematical structure of the Hermitian kinetic energy operator proposed by von Roos [2], which characterises the most of those used in the literature [13–18].

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Recently, a q-deformed Schrödinger equation associated with a PDM [19–30] has been explored in the context of a generalised translation operator related to a non-additive algebraic structure [31,32], which arose by the non-extensive statistical mechanics [33]. The latter has a wide range of applicability for characterising a variety of phenomena (non-ergodicity, long-range interactions, etc.), that justify it as an extended theory where standard statistical mechanics can be considered as a special case. The term non-extensive is conceivable as the nonlinear growing of physical magnitudes of the system with increasing its degrees of freedom. Nonetheless, subsequent developments in the mathematical structure of non-extensive statistical mechanics implied a subtle use of this term, for referring to formalisms that use such structures [31,32]. In this work we follow this convention.

The letter is organised as follows: First we present a preliminary about the deformed Schrödinger equation (DSE) from the general kinetic term introduced by von Roos, which is used to model a particle with an effective position-dependent mass. Then, we introduce our model that is a special case of the DSE and whose solutions are a generalisation of the ordinary plane waves. These deformed plane waves recover the usual plane waves when the deformation parameter $\gamma \propto 1-q$ tends to zero. Second, we generalise the Bloch theorem for potentials that have a deformed translational invariance, and we obtain the exact solutions for two models employed in the literature of solid-state physics: the Dirac potential and the Kronig-Penney one [34]. For these models we study the energy bands, the probability distributions and the density of states, and we compare them with the non-deformed case. We illustrate this with two applications: semiconductor phase transitions and continuous distribution of defects. Last, we outline some conclusions and give some futures possibilities to be investigated in this scenario. In the following, we present a series of behaviors to exemplify the differences between the usual potentials and the quasi-periodic potentials.

Deformed Schrödinger equation for PDM systems. – In this section, we present a review of how a non-additive formalism in quantum mechanics can be used for describing a PDM system. The formalism is based on a q-algebraic structure that emerges from non-extensive statistical mechanics.

Review of the q-deformed algebra. The q-exponential is a deformation of the ordinary exponential function, defined by $\exp_q u \equiv [1+(1-q)u]_+^{1/(1-q)}$ with $[u]_+ \equiv \max\{u,0\}$. The inverse function of the q-exponential is the q-logarithm function, given by $\ln_q u \equiv \frac{u^{1-q}-1}{1-q}$. In the limit $q \to 1$, the ordinary exponential and logarithm functions are recovered, $\exp_1 x = \exp x$ and $\ln_1 x = \ln x$. These functions satisfy the properties $\exp_q(a)\exp_q(b) = \exp_q(a \oplus_q b)$, $\exp_q(a)/\exp_q(b) = \exp_q(a \ominus_q b)$, $\ln_q(ab) = \ln_q(a) \oplus_q \ln_q(b)$ and $\ln_q(a/b) = \ln_q(a) \ominus_q \ln_q(b)$, where the symbol $\oplus_q$ represents the q-addition operator defined by $a \oplus_q b \equiv a+b+(1-q)ab$, and $\ominus_q$ represents the q-subtraction, $a \ominus_q b \equiv \frac{a-b}{1+(1-q)b} (b \neq \frac{1}{q-1})$ [31,32].

A q-deformed calculus has been introduced from the deformed differential

$$\mathrm{d}_q u \equiv \lim_{u' \to u} u' \ominus_q u = \frac{\mathrm{d}u}{1+(1-q)u}. \tag{1}$$

The definition of a deformed variable u_q (also named deformed q-number),

$$u_q \equiv \frac{\ln[1+(1-q)u]}{1-q} = \ln[\exp_q(u)], \tag{2}$$

implies $\mathrm{d}_q u = \mathrm{d}u_q$, *i.e.*, the *deformed differential* of an ordinary variable u coincides with the ordinary differential of a *deformed variable* u_q. In this way, the q-derivative operator is defined by

$$D_q f(u) \equiv \lim_{u' \to u} \frac{f(u')-f(u)}{u' \ominus_q u} = [1+(1-q)u]\frac{\mathrm{d}f(u)}{\mathrm{d}u}, \tag{3}$$

being the q-exponential an eigenfunction, $D_q \exp_q u = \exp_q u$. Recently, Weberszpil *et al.* [35] have shown a connection between the deformed derivative (3) and the Hausdorff derivative operator associated with fractional calculus. The deformed derivative operator (3) can be seen as the variation of the function $f(u)$ with respect to a nonlinear variation of the independent variable u, *i.e.*, $D_q f(u) = \mathrm{d}f(u)/\mathrm{d}u_q$, where the deformed second derivative satisfies

$$D_q^2 f(u) = [1+(1-q)u]\frac{\mathrm{d}}{\mathrm{d}u}\left\{[1+(1-q)u]\frac{\mathrm{d}f}{\mathrm{d}u}\right\}. \tag{4}$$

Non-additive quantum formalism for PDM. In the approach of quantum systems with PDM the mass and the linear momentum are non-commuting operators, which gives place to the ordering problem for defining the kinetic energy operator. There are several ways to define an Hermitian kinetic energy operator $\hat{K}$, and a general form was proposed by von Roos [2]

$$\begin{aligned}\hat{K} = \frac{1}{4}\big\{&[m(\hat{x})]^{-\eta}\hat{p}[m(\hat{x})]^{-1+\eta+\nu}\hat{p}[m(\hat{x})]^{-\nu} \\ &+[m(\hat{x})]^{-\nu}\hat{p}[m(\hat{x})]^{-1+\eta+\nu}\hat{p}[m(\hat{x})]^{-\eta}\big\},\end{aligned} \tag{5}$$

from which some of the most prominent kinetic energy operators in the literature can be obtained: Ben Daniel and Duke (BDD) [13] ($\eta=\nu=0$), Gora and Williams (GW) [14] ($\eta=1$, $\nu=0$), Zhu and Kroemer (ZK) [15] ($\eta=\nu=\frac{1}{2}$), Li and Kuhn (LK) [16] ($\eta=0, \nu=\frac{1}{2}$). Morrow *et al.* [17] have shown that the case $\eta=\nu$ satisfies the conditions of continuity of the wave function at the boundaries of a heterojunction in crystals. In particular, Mustafa and Mazharimousavi [18] have shown that the case $\eta=\nu=\frac{1}{4}$, named ordering MM, allows the mapping of a quantum Hamiltonian with PDM into a Hamiltonian with constant mass by means of a point canonical transformation. Considering the quantum Hamiltonian

$$\hat{H}(\hat{x},\hat{p}) = \frac{1}{2}[m(\hat{x})]^{-\frac{1}{4}}\hat{p}[m(\hat{x})]^{-\frac{1}{2}}\hat{p}[m(\hat{x})]^{-\frac{1}{4}} + V(\hat{x}), \tag{6}$$

the time-independent Schrödinger equation $\hat{H}|\psi\rangle = E|\psi\rangle$ in the representation $\{|\hat{x}\rangle\}$ is

$$\left[-\frac{\hbar^2}{2m_0}\sqrt[4]{\frac{m_0}{m(x)}}\frac{\mathrm{d}}{\mathrm{d}x}\sqrt{\frac{m_0}{m(x)}}\frac{\mathrm{d}}{\mathrm{d}x}\sqrt[4]{\frac{m_0}{m(x)}}+V(x)\right]\psi(x) = E\psi(x), \tag{7}$$

where $\psi(x)$ is the wave function solution and $m(x) = m_0$ recovers the standard Schrödinger equation. By defining the mass function,

$$m(x) = \frac{m_0}{(1+\gamma x)^2}, \tag{8}$$

with $\gamma = (1-q)/L$ and L a characteristic length, the field $\varphi(x) = (\sqrt{1+\gamma x})\psi(x)$ obeys a time-independent *deformed Schrödinger wave equation* (DSE) [19]

$$-\frac{\hbar^2}{2m_0}D_\gamma^2\varphi(x) + V(x)\varphi(x) = E\varphi(x), \tag{9}$$

where $D_\gamma = (1+\gamma x)\frac{\mathrm{d}}{\mathrm{d}x}$ has a structure similar to that of q-derivative (3). Equation (9) is equivalent to a Schrödinger-like equation for $\varphi(x)$ expressed in terms of the non-Hermitian quantum Hamiltonian operator $\hat{H}_\gamma = \frac{1}{2m_0}\hat{p}_\gamma^2 + V(\hat{x})$ and $\hat{p}_\gamma \equiv (1+\gamma\hat{x})\hat{p} = -\mathrm{i}\hbar D_\gamma$ a deformed non-Hermitian momentum operator, which satisfies the commutator relation $[\hat{x}, \hat{p}_\gamma] = \mathrm{i}\hbar(\hat{1} + \gamma\hat{x})$. The wave functions $\varphi(x)$ are normalised by means of a deformed inner product $\langle\varphi_1|\varphi_2\rangle = \int_{x_i}^{x_f}\varphi_1^*(x)\varphi_2(x)\mathrm{d}_\gamma x$ where $\mathrm{d}_\gamma x = \mathrm{d}x/(1+\gamma x)$. So, the probability density results

$$\rho_\gamma(x) = \frac{\varphi^*(x)\varphi(x)}{1+\gamma x}. \tag{10}$$

Using the change of variable $x \to x_\gamma = \gamma^{-1}\ln(1+\gamma x)$, eq. (9) can be recasted in the deformed space x_γ as

$$-\frac{\hbar^2}{2m_0}\frac{\mathrm{d}^2\phi(x_\gamma)}{\mathrm{d}x_\gamma^2} + U(x_\gamma)\phi(x_\gamma) = E\phi(x_\gamma), \tag{11}$$

where $\phi(x_\gamma) = \varphi(x(x_\gamma))$ and $U(x_\gamma) = V(x(x_\gamma))$ are the field and the potential in the deformed space. Thus, the wave equation for the field $\psi(x)$ of a system with a PDM (8) in the standard space $\{|\hat{x}\rangle\}$ is mapped into an equation for the field $\phi(x_\gamma)$ in a deformed space $\{|\hat{x}_\gamma\rangle\}$.

The free particle solution ($V(x) = 0$) in the representation $\{|\hat{x}\rangle\}$ is, as expected, an imaginary deformed exponential $\varphi(x) = A_0\mathrm{e}^{\pm\mathrm{i}k\gamma^{-1}\ln(1+\gamma x)} = A_0\left[\exp_q\left(\frac{x}{L}\right)\right]^{\pm\mathrm{i}kL}$, with $k = \sqrt{2m_0E}/\hbar$. It recovers the usual exponential for $q \to 1$ ($\gamma = 0$). In the deformed space basis $\{|\hat{x}_\gamma\rangle\}$, the wave function has the usual form $\phi(x_\gamma) = A_0\mathrm{e}^{\pm\mathrm{i}kx_\gamma}$. As in the usual case ($\gamma = 0$), the function $\varphi(x)$ is also not normalised. Also, a wave packet can be defined from the deformed Fourier transform

$$\varphi(x) = \int_{-\infty}^{+\infty}\widetilde{A}(k)\mathrm{e}^{\mathrm{i}k\gamma^{-1}\ln(1+\gamma x)}\mathrm{d}k, \tag{12}$$

where $\widetilde{A}(k)$ is the distribution function of the wave vectors k. Analogously, the corresponding wave packet in the representation of the deformed space basis $\{|\hat{x}_\gamma\rangle\}$ is $\phi(x_\gamma) = \varphi(x(x_\gamma)) = (\sqrt{1+\gamma x})\psi(x(x_\gamma)) = \int_{-\infty}^{+\infty}\widetilde{A}(k)\mathrm{e}^{\mathrm{i}kx_\gamma}\mathrm{d}k$. From the Plancherel theorem, we have

$$\begin{aligned}\widetilde{A}(k) &= \frac{1}{2\pi}\int_{-\infty}^{+\infty}\phi(x_\gamma)\mathrm{e}^{-\mathrm{i}kx_\gamma}\mathrm{d}x_\gamma \\ &= \frac{1}{2\pi}\int_{-\infty}^{+\infty}\frac{\varphi(x)}{1+\gamma x}\mathrm{e}^{-\mathrm{i}k\gamma^{-1}\ln(1+\gamma x)}\mathrm{d}x \\ &= \frac{1}{2\pi}\int_{-\infty}^{+\infty}\frac{\psi(x)}{\sqrt{1+\gamma x}}\mathrm{e}^{-\mathrm{i}k\gamma^{-1}\ln(1+\gamma x)}\mathrm{d}x. \end{aligned}\tag{13}$$

Dirac delta and Kronig-Penney potentials. – As an application of the formalism presented in the previous section, we obtain the solutions of the DSE (9) for the Dirac delta potential and a combination of them that can be used to represent the potential of a crystal lattice with defects.

Dirac delta potential. Consider a particle with a PDM and a energy E under the influence of a delta potential $V(x) = -\alpha\delta(x - x_\mathrm{c})$, where α (area of the potential barrier) is a positive constant of *energy* $\times$ *length* dimensions and x_c is the position for which the potential diverges. The DSE (9) becomes

$$-\frac{\hbar^2}{2m_0}D_\gamma^2\varphi(x) - \alpha\delta(x-x_\mathrm{c})\varphi(x) = E\varphi(x). \tag{14}$$

As in the standard case, the wave function satisfies the continuity of the lateral limits, *i.e.*, $\lim_{x\to y^+}\varphi(x) = \lim_{x\to y^-}\varphi(x)\ \forall x$, with the particularity that by integrating eq. (14) between $x_\mathrm{c} - \epsilon$ and $x_\mathrm{c} + \epsilon$ with $\epsilon \to 0$, we obtain

$$\begin{aligned}&\frac{\hbar^2}{2m_0}\int_{x_\mathrm{c}-\epsilon}^{x_\mathrm{c}+\epsilon}[z(x)]^2\frac{\mathrm{d}^2\varphi(x)}{\mathrm{d}x^2}\mathrm{d}x + \frac{\hbar^2\gamma}{2m_0}\int_{x_\mathrm{c}-\epsilon}^{x_\mathrm{c}+\epsilon}z(x)\frac{\mathrm{d}\varphi(x)}{\mathrm{d}x}\mathrm{d}x = \\ &-\alpha\int_{x_\mathrm{c}-\epsilon}^{x_\mathrm{c}+\epsilon}\delta(x-x_\mathrm{c})\varphi(x)\mathrm{d}x,\end{aligned}\tag{15}$$

with $z(x) = 1 + \gamma x$. Applying integration by parts in the first two integrals, we arrive at

$$\lim_{\epsilon\to 0}\left(\frac{\mathrm{d}\varphi(x)}{\mathrm{d}x}\bigg|_{x_\mathrm{c}+\epsilon} - \frac{\mathrm{d}\varphi(x)}{\mathrm{d}x}\bigg|_{x_\mathrm{c}-\epsilon}\right) = -\frac{2m(x_\mathrm{c})\alpha}{\hbar^2}\varphi(x_\mathrm{c}). \tag{16}$$

For bound states ($E < 0$) and $1 + \gamma x_\mathrm{c} > 0$, the wave function is

$$\varphi(x) = \begin{cases} B_0\mathrm{e}^{-\kappa\gamma^{-1}\ln(1+\gamma x)}, & x > x_\mathrm{c}, \\ B_0\mathrm{e}^{\kappa\gamma^{-1}\ln(1+\gamma x)}, & -1/\gamma < x < x_\mathrm{c}, \\ 0, & x < -1/\gamma, \end{cases} \tag{17}$$

with $B_0 = \frac{1}{\hbar}\sqrt{\frac{m_0\alpha}{1+\gamma x_\mathrm{c}}}$ the normalisation constant and $E = -\hbar^2\kappa^2/2m_0 = -m(x_\mathrm{c})\alpha^2/2\hbar^2$ the energy. The wave function $\varphi(x)$ is zero for $x < -1/\gamma$ due to the cut-off of the q-exponential function.

For unbound states ($E > 0$), the reflection and transmission coefficients are given respectively, by $r = [1 + \frac{2\hbar^2E}{m(x_\mathrm{c})\alpha^2}]^{-1}$ and $t = [1 + \frac{m(x_\mathrm{c})\alpha^2}{2\hbar^2E}]^{-1}$.

Periodic potential with a defect: deformed Bloch theorem. Now we consider a one-dimensional model for a solid in which the ions are fixed but have a defect so that the potential is quasi-periodic and satisfies the condition (that we called non-additive translational invariance)

$$V(x) = V(x + a + \gamma xa), \tag{18}$$

which expresses that $V(x)$ is invariant under deformed spatial translations. The argument on the right-hand side of V can be written as a q-sum: $x + a + \gamma xa = L[(x/L) \oplus_q (a/L)]$. In order to discuss this problem more formally, we employ a deformed translation operator $\hat{T}_\gamma(a)$ defined by

$$\hat{T}_\gamma(a)\varphi(x) = \varphi(x + a + \gamma xa), \tag{19}$$

that is originally associated with the formulation of the deformed Schrödinger equation (9) [19,20]. The point here is that for potentials of the type (18), the operators $\hat{H}_\gamma$ and $\hat{T}_\gamma(a)$ commute. In fact, since

$$\begin{aligned}\hat{p}_\gamma \hat{T}_\gamma(a)\varphi(x) &= -\mathrm{i}\hbar(1+\gamma x)\frac{\mathrm{d}}{\mathrm{d}x}\varphi(x + a + \gamma xa) \\ &= -\mathrm{i}\hbar[1 + \gamma(x + a + \gamma xa)]\frac{\mathrm{d}\varphi}{\mathrm{d}x}\Big|_{x+a+\gamma xa} \\ &= \hat{T}_\gamma(a)\hat{p}_\gamma\varphi(x) \end{aligned} \tag{20}$$

and

$$\begin{aligned} V(\hat{x})\hat{T}_\gamma(a)\varphi(x) &= V(x)\varphi(x + a + \gamma xa) \\ &= V(x + a + \gamma xa)\varphi(x + a + \gamma xa) \\ &= \hat{T}_\gamma(a)V(\hat{x})\varphi(x), \end{aligned} \tag{21}$$

so we have $[\hat{H}_\gamma, \hat{T}_\gamma(a)] = 0$. Hence, the eigenfunctions of $\hat{T}_\gamma(a)$, that we called deformed Bloch states, are also eigenfunctions of $\hat{H}_\gamma$ for quasi-periodic potentials of the type (18). Then, the deformed Bloch states are given by

$$\varphi(x) = \mathrm{e}^{\mathrm{i}s\gamma^{-1}\ln(1+\gamma x)}u_s(x), \tag{22}$$

where $u_s(x) = u_s(x + a + \gamma xa)$. Indeed,

$$\begin{aligned}\hat{T}_\gamma(a)\varphi(x) &= \mathrm{e}^{\mathrm{i}s\gamma^{-1}\ln[1+\gamma(x+a+\gamma xa)]}u_s(x + a + \gamma xa) \\ &= \mathrm{e}^{\mathrm{i}s\gamma^{-1}\ln(1+\gamma a)}\varphi(x), \end{aligned} \tag{23}$$

where the factor $\mathrm{e}^{\mathrm{i}s\gamma^{-1}\ln(1+\gamma a)}$ is the eigenvalue of the operator $\hat{T}_\gamma(a)$ for the deformed Bloch states (22). The usual case $\varphi(x) = \mathrm{e}^{\mathrm{i}sa}u_s(x)$ is recovered for $\gamma \to 0$. Additionally, it is straightforwardly verified that the deformed Bloch states satisfy the q-inner product

$$\int_{x_i}^{x_f}\frac{\varphi^*(x)\varphi(x)}{1+\gamma x}\mathrm{d}x = \int_{x_i}^{x_f}\frac{[\hat{T}_\gamma(a)\varphi(x)]^*[\hat{T}_\gamma(a)\varphi(x)]}{1+\gamma x}\mathrm{d}x = \int_{x_i}^{x_f}\frac{\varphi^*(x + a + \gamma xa)\varphi(x + a + \gamma xa)}{1+\gamma x}\mathrm{d}x. \tag{24}$$

Thus, the steps (18)–(24) can be considered as the deformed version of the Bloch theorem in the context of non-extensive statistical mechanics.

Deformed Dirac-Kronig-Penney potential. We consider a modified version of the Dirac-Kronig-Penney model [34] with the potential given by

$$V(x) = \alpha\sum_{n=-\infty}^{+\infty}\delta\left(\frac{x - a_n}{1 + \gamma a_n}\right), \tag{25}$$

where $a_n = \gamma^{-1}[(1 + \gamma a)^n - 1] = L\ln_q[\exp_q^n(a/L)]$ is the position of the ions in the crystal lattice. It is straightforwardly verified that the potential (25) satisfies (18). For $\gamma a > 0$ ($-1 < \gamma a < 0$), the separation distance between two consecutive crystal ions, $\lambda_n = a_n - a_{n-1}$, increases (decreases) with n. From the properties of the Dirac delta function, the n-th potential barrier area changes by a factor of $(1+\gamma a)^n$. The non-additive translational invariance introduces physically a deformation of the lattice, that can model a non-periodic crystal with sites localised in $a_n\,\forall n$ with a potential barrier area $\alpha_n = \alpha(1 + \gamma a)^n$. The solution of eq. (9) in the interval $0 \le x \le a$ is

$$\varphi(x) = A\sin\left[\frac{k}{\gamma}\ln(1+\gamma x)\right] + B\cos\left[\frac{k}{\gamma}\ln(1+\gamma x)\right], \tag{26}$$

with $E = \hbar^2k^2/2m_0$. From the deformed Bloch functions, the solution immediately to the left of $x = 0$ (*i.e.*, in the interval $-a/(1 + \gamma a) \le x \le 0$) is

$$\begin{aligned}\varphi(x) = \mathrm{e}^{-\mathrm{i}sa_\gamma}\Bigg\{&A\sin\left[\frac{k}{\gamma}\ln(1+\gamma x) + \frac{k}{\gamma}\ln(1+\gamma a)\right] \\ &+B\cos\left[\frac{k}{\gamma}\ln(1+\gamma x) + \frac{k}{\gamma}\ln(1+\gamma a)\right]\Bigg\}, \end{aligned} \tag{27}$$

in which $a_\gamma = \gamma^{-1}\ln(1 + \gamma a)$. From the continuity of the wave function $\varphi(x)$ and discontinuity of the derivative $\mathrm{d}\varphi(x)/\mathrm{d}x$ (eq. (16)), both at $x = 0$, we obtain, respectively,

$$B\left\{\mathrm{e}^{\mathrm{i}sa_\gamma} - \cos\left[\frac{k}{\gamma}\ln(1+\gamma a)\right]\right\} = A\sin\left[\frac{k}{\gamma}\ln(1+\gamma a)\right],$$

and

$$\left\{B\sin\left[\frac{k}{\gamma}\ln(1+\gamma a)\right] - A\cos\left[\frac{k}{\gamma}\ln(1+\gamma a)\right]\right\}k\mathrm{e}^{\mathrm{i}sa_\gamma} + kA = \frac{2m_0\alpha}{\hbar^2}B. \tag{28}$$

Solving the above equations we found the dispersion relationship

$$\begin{aligned}\cos\left[\frac{s}{\gamma}\ln(1+\gamma a)\right] &= \cos\left[\frac{k}{\gamma}\ln(1+\gamma a)\right] \\ &+\left(\frac{\beta}{ka}\right)\sin\left[\frac{k}{\gamma}\ln(1+\gamma a)\right], \end{aligned} \tag{29}$$

where $\beta = m_0\alpha a/\hbar^2$ is the scattering power. Considering the deformed space, eq. (29) can be rewritten more compactly as $\cos(sa_\gamma) = \cos(ka_\gamma) + \beta_\gamma\frac{\sin(ka_\gamma)}{ka_\gamma}$, with

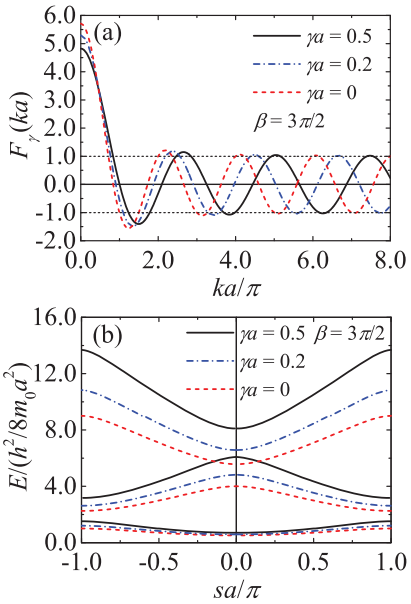

Fig. 1: (a) Function $F_\gamma(ka) = \cos[k\gamma^{-1}\ln(1+\gamma a)] + (\beta/ka)\sin[k\gamma^{-1}\ln(1+\gamma a)]$ for the usual case $\gamma = 0$ (dashed line), $\gamma = 0.2$ (dash-dotted line) and $\gamma = 0.5$ (solid line), with a standard scattering power $\beta = m_0\alpha a/\hbar^2 = 3\pi/2$. (b) Reduced scheme of the energy bands and the gaps.

$\beta_\gamma = \frac{a_\gamma}{a}\beta$. Similar to the standard case, the possible wave vectors for bound states, and therefore the allowed energy bands, satisfy the condition $-1 \leq F_\gamma(ka) \leq 1$ with $F_\gamma(ka) = \cos[k\gamma^{-1}\ln(1+\gamma a)] + (\beta/ka)\sin[k\gamma^{-1}\ln(1+\gamma a)]$. The limit $\beta \to \infty$ recovers the problem of a particle confined in a one-dimensional box where the wave vectors are $k_n = n\pi/a_\gamma$, and the energies are $E_n = \hbar^2\pi^2 n^2/2m_0 a_\gamma^2$ as obtained in ref. [19]. Figure 1(a) shows the function $F_\gamma(ka)$ for $\beta = 3\pi/2$ and different values of the deformation parameter γa. From the eq. (22) and the deformed periodic boundary condition $\varphi(x + a_N + \gamma x a_N) = \varphi(x)$, with $N \gg 1$, we obtain $\mathrm{e}^{Nis\gamma^{-1}\ln(1+\gamma a)} = 1$. Thereby, $s = 2\pi j/Na_\gamma$ with $j = 0, 1, 2, \ldots, N-1$. In this sense, there are N possible states for each energy band. The effect of the deformation parameter γ on the allowed energies and band energy gaps are illustrated in table 1. Figure 1(b) shows the reduced scheme of the energy spectrum obtained from the numerical solution of $\cos(2\pi j/N) = F_\gamma(ka)$ for different values of γa. It can be seen that the allowed energy levels and gaps increase as γa increases. From the definition of the effective mass, $1/m^*_{\text{eff.}} = 1/\hbar^2(\partial^2 E/\partial s^2)$, we see that $m^*_{\text{eff.}}$ increases when γa decreases.

By means of eq. (28), we can rewrite the wave function in the form

$$\varphi(x) = C\left\{\sin\left[\frac{k}{\gamma}\ln(1+\gamma x)\right] - \mathrm{e}^{-is\gamma^{-1}\ln(1+\gamma a)} \times \sin\left[\frac{k}{\gamma}\ln\left(\frac{1+\gamma x}{1+\gamma a}\right)\right]\right\}, \quad (30)$$

in which C is a normalisation constant. Considering the probability density (10) and the normalisation condition $\lim_{N\to\infty}\int_0^{a_N}\rho_\gamma(x)\mathrm{d}x = 1$ in the limit of infinite sites, one obtains from the software `Mathematica` [36] $N|C|^2 = \{a_\gamma[1-\cos(sa_\gamma)\cos(ka_\gamma)]\}^{-1}$, and then,

$$N\rho_\gamma(x) = \frac{\gamma}{\ln(1+\gamma a)[1-\cos(sa_\gamma)\cos(ka_\gamma)]}\frac{1}{1+\gamma x} \times\left\{\sin^2\left[\frac{k}{\gamma}\ln(1+\gamma x)\right] + \sin^2\left[\frac{k}{\gamma}\ln\left(\frac{1+\gamma x}{1+\gamma a}\right)\right] -2\cos(sa_\gamma)\sin\left[\frac{k}{\gamma}\ln(1+\gamma x)\right] \times\sin\left[\frac{k}{\gamma}\ln\left(\frac{1+\gamma x}{1+\gamma a}\right)\right]\right\}. \quad (31)$$

In fig. 2 we show the probability density functions in the cell $0 < x < a$ for different values of γa at the top and bottom of the first three energy bands (*i.e.*, $ka = \pi, 2\pi, 3\pi$) with $\beta = 3\pi/2$. The usual case $\gamma a = 0$ is shown for comparison. For $\gamma \neq 0$ it is observed that the points $x = 0$ and $x = a$ are no longer nodes. The density of states $g(E) = \frac{2}{\pi}\frac{\partial k}{\partial E}$ for the dispersion relation (29) becomes

$$g(E) = \frac{1}{a\varepsilon_0}\sqrt{\frac{\varepsilon_0}{E}}\frac{1}{\sin(sa_\gamma)}\left\{\sin(\theta_\gamma(E)) +\beta_\gamma\left[\frac{\sin(\theta_\gamma(E))}{\theta^2_\gamma(E)} - \frac{\cos(\theta_\gamma(E))}{\theta_\gamma(E)}\right]\right\}, \quad (32)$$

with $\theta_\gamma(E) = \pi\frac{a_\gamma}{a}\sqrt{\frac{E}{\varepsilon_0}}$ and $\varepsilon_0 = \frac{\hbar^2}{8m_0a^2}$. Figure 3 shows the density of states for the first energy band and for the values of $\gamma a = 0, 0.2, 0.5$. We note that the distribution shifts to the right as γ increases, similar to the effect of an electric field on a Fermi surface for free electrons.

Physical relevance: Phase transitions and defects. From fig. 1 and table 1 we see that the deformed Dirac-Kronig-Penney potential presents an energy band gap corresponding to a semiconductor, where the deformation parameter γ produces a displacement (5th and 6th columns) and a width variation (2th–4th columns) of the energy gaps, but maintaining the nature of a direct band gap. Table 1 expresses a transition from a semiconductor, having an increasing band gap with γa from 0 to 0.5, into other more insulators. Putting values, if a is of the order of the Bohr radio and m_0 the electron mass we have that $h^2/8m_0a^2 \approx 1.342\,\text{eV}$, so the first bands gaps (5th column of table 1) adjust well with the ones corresponding to copper cadmium ($1.342 \times 1.250 \approx 1.7\,\text{eV}$) and zinc telluride ($1.342 \times 1.657 \approx 2.25\,\text{eV}$) at room temperature.

A non-uniform potential strength allows to model a lattice provided with different atomic potentials, as was reported in a generalised Dirac-Kronig-Penney model [37], and a non-uniform distribution of sites characterises a lattice with defects. These two joint effects are relevant in continuous distribution of defects when the lattice spacing goes to zero, requiring potential strengths of arbitrarily small magnitude. This is the case of real crystalline solids where the density of defects is very high,

Table 1: The allowed energies E and the first two band energy gaps (both in units of $h^2/8m_0a^2$) of a PDM particle for different values of γa and for a scattering power $\beta = 3\pi/2$.

γa	Range of E in band 1	Range of E in band 2	Range of E in band 3	First band gap	Second band gap
0	0.514 to 1.000	2.250 to 4.000	5.571 to 9.000	1.250	1.571
0.2	0.588 to 1.203	2.621 to 4.812	6.572 to 10.827	1.418	1.760
0.5	0.696 to 1.520	3.177 to 6.081	8.105 to 13.682	1.657	2.024

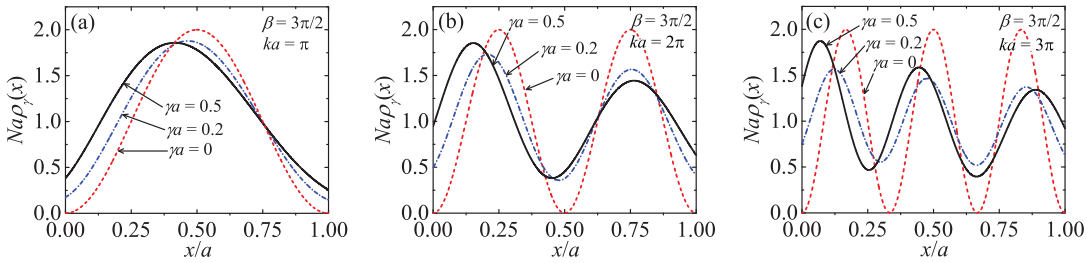

Fig. 2: (a) Dimensionless probability distribution functions (31) for (a) $ka = \pi$, (b) 2π and (c) 3π and the deformation parameters $\gamma a = 0$ (usual case), 0.2 and 0.5 with a scattering power $\beta = 3\pi/2$.

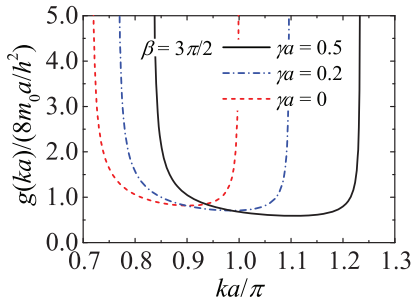

Fig. 3: Density of states for the first energy band and values of the deformation parameter $\gamma a = 0$, 0.2 and 0.5.

with 10^8–10^{10} mm/mm^3 number of dislocations. From the modified Dirac delta potential (25) this situation can be modeled for $\gamma a < 0$ and for sites a_n with $n > 0$. Let us consider $\gamma a = -0.5$ ($\gamma < 0$). Then, the strength potential satisfies $\alpha(0.5)^n \to 0$ for $n \to \infty$ while the sites $a_n = \frac{(0.5)^n - 1}{\gamma} \to -\frac{1}{\gamma} > 0$ for $n \to \infty$, that correspond to a lattice with defects accumulated around $x = -\frac{1}{\gamma}$ for $n \to \infty$. Within the range $n = 10^8$–10^{10} of number of sites the relative lattice spacing $\lambda_n\gamma$ results between $(0.5)^{10^{10}}$–$(0.5)^{10^7}$, thus representing a continuous density of defects.

Conclusions. – From a generalised version of the Schrödinger equation for PDM systems inspired in non-exstensive statistics, we have addressed the problem of one-dimensional periodic potentials in a deformed lattice with non-periodically localised sites. We have obtained a deformed version of the Bloch theorem, whose deformed Bloch states satisfy a non-additive translational invariance that is compatible with the deformed lattice assumed. In all the cases the standard definitions and concepts are recovered when the deformation goes to zero ($\gamma \to 0$).

We have illustrated the formalism presented with two examples: the Dirac delta and the Kroning-Penney potentials. For the Dirac potential we have obtained the deformed eigenstates along with the reflection and transmission coefficients. In the case of the Kronig-Penney model we have considered a modified version, corresponding to a deformed lattice having a non-uniform neighbour distance.

We found an asymmetry of the probability distribution functions of the eigenfunctions (see fig. 2), while the reduced scheme of the energy bands presents a displacement and an increase in the band gaps (fig. 1(b) and table 1), that can be interpreted as a phase transition to a more insulator behavior. The density of states exhibits a shift to the right as a consequence of the position-dependent mass chosen $m(x) = m_0/(1+\gamma x)^2$. Complementarily, we also have discussed the representation of a lattice with a continuous distribution of defects and potential strengths turning out to be arbitrarily small, being both effects controlled by the dimensionless deformation parameter γa.

* * *

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Appendix: deformed Kronig-Penney model in reciprocal lattice space. – The dispersion ratio for the Kronig-Penney model can be obtained from the reciprocal lattice space. Considering the

field $\varphi(x)$ and the potential expressed in a deformed Fourier series analogous to the corresponding transform (12) $V(x) = \sum_{G_n} \widetilde{V}(G_n) \mathrm{e}^{\mathrm{i}G_n\gamma^{-1}\ln(1+\gamma x)}$, $\varphi(x) = \sum_s \widetilde{A}(s)\mathrm{e}^{\mathrm{i}s\gamma^{-1}\ln(1+\gamma x)}$ and replacing in (9), we obtain

$$(\zeta_s - E)\widetilde{A}(s) + \sum_{G_n} \widetilde{V}(G_n)\widetilde{A}(s - G_n) = 0, \tag{A.1}$$

where $\zeta_s = \hbar^2 s^2/2m_0$. Equation (A.1) has the same form as the usual case due to the non-additive periodicity of the potential, while (eq. (18)) the deformed reciprocal lattice vectors for the one-dimensional solid are given by $G_n = 2\pi n/a_\gamma$ with n integer and a_γ the new lattice parameter. The coefficients of the series for potential (25) are

$$\widetilde{V}(G_n) = \frac{\alpha}{a_\gamma} \sum_{n=-\infty}^{+\infty} \int_{x'}^{x'+a+\gamma x' a} \delta\left(\frac{x - a_n}{1+\gamma a_n}\right) \times \mathrm{e}^{-\mathrm{i}G_n\gamma^{-1}\ln(1+\gamma x)} \mathrm{d}_\gamma x, \tag{A.2}$$

with x' an arbitrary position, that is equals to

$$\begin{aligned}\widetilde{V}(G_n) &= \frac{\alpha}{a_\gamma} \sum_{n=-\infty}^{+\infty} \int_{x'_\gamma}^{x'_\gamma + a_\gamma} \delta\left(\frac{\mathrm{e}^{\gamma x_\gamma} - (1+\gamma a_n)}{\gamma(1+\gamma a_n)}\right) \\ &\quad \times \mathrm{e}^{-\mathrm{i}G_n x_\gamma} \mathrm{d}x_\gamma \\ &= \frac{\alpha}{a_\gamma},\end{aligned} \tag{A.3}$$

where $x'_\gamma = \gamma^{-1}\ln(1+\gamma x')$, and where we have used $\delta(f(u)) = \sum_{u_0} \frac{\delta(u-u_0)}{|f'(u_0)|}$ $(f(u_0) = 0)$. Consequently, eq. (A.1) for Dirac-Kronig-Penney potential becomes

$$(\zeta_s - E)\widetilde{A}(s) + \sum_{G_n} \frac{\alpha}{a_\gamma}\widetilde{A}(s - G_n) = 0. \tag{A.4}$$

Following the same path as in ref. [38], it is immediate to show that (A.4) leads to the dispersion relation

$$\cos(sa_\gamma) = \cos(ka_\gamma) + \frac{m_0\alpha}{2\hbar^2 k}\sin(ka_\gamma), \tag{A.5}$$

with $E = \hbar^2 k^2/2m_0$ and $\beta = m_0\alpha a/2\hbar^2$ is the scattering power, in accordance with the Dirac-Kronig-Penney potential, differing from eq. (29) by a factor of $\frac{1}{2}$.

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