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Displacement operator for quantum systems with position-dependent mass

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A translation operator is introduced to describe the quantum dynamics of a position-dependent mass particle in a null or constant potential. From this operator, we obtain a generalized form of the momentum operator as well as a unique commutation relation for $\hat{x}$ and $\hat{p}_\gamma$. Such a formalism naturally leads to a Schrödinger-like equation that is reminiscent of wave equations typically used to model electrons with position-dependent (effective) masses propagating through abrupt interfaces in semiconductor heterostructures. The distinctive features of our approach are demonstrated through analytical solutions calculated for particles under null and constant potentials like infinite wells in one and two dimensions and potential barriers.

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The concept of noncommutative coordinates as a way of removing divergences in field theories through a universal invariant length parameter was originally proposed by Heisenberg [1]. This idea led to space-time quantization [2], where a noncommutative space operator is defined to allow for the development of a theory invariant under Lorentz transformation, but not invariant under translations. Accordingly, the last property leads to continuous space-time coordinates. Since then, the need for a fundamental length scale became evident in different areas of physics, such as relativity [3], string theory [4], and quantum gravity [5]. In the particular case of quantum mechanics, this minimum length scale yields a modification in the position momentum commutation relationship [6–9].

Previous studies have shown that the modification of canonical commutation relations or any modification in the underlying space typically results in a Schrödinger equation with a position-dependent mass [10]. This approach has been rather effective in the description of electronic properties of semiconductor [11] and quantum dots [12]. Under this framework, mass is turned into an operator that does not commute with the momentum operator. This fact immediately raises the problem of the ordering of these operators in the kinetic energy operator [13]. In this Rapid Communication, we introduce the concept of nonadditive spatial displacement in the Hilbert space. This property not only changes the commutation relation for position and momentum, which leads to a modified uncertainty relation, but also reveals a Schrödinger-like differential equation that can be interpreted in terms of a particle with position-dependent mass, leading to a natural derivation of the kinetic operator for such problems.

Consider a well-localized state around x that can be changed to another well-localized state around $x + a + \gamma ax$ with all the other physical properties unchanged, where the parameter γ is the inverse of a characteristic length that determines the mixing between the displacement and the original position state. For $\gamma \neq 0$, the displacement depends explicitly on the position of the system, while $\gamma = 0$ corresponds to a standard translation. This process can be mathematically expressed in terms of the operator $\mathcal{T}_\gamma(a)$ as

$$\mathcal{T}_\gamma(a)|x\rangle = |x + a + \gamma ax\rangle. \quad (1)$$

The composition of displacements through $\mathcal{T}_\gamma$ in terms of two successive infinitesimal translations results in

$$\mathcal{T}_\gamma(dx')\mathcal{T}_\gamma(dx'') = \mathcal{T}_\gamma(dx' + dx'' + \gamma dx'dx''), \quad (2)$$

which clearly shows the nonadditivity characteristic of the operator. It is also important to note that the inverse operator is given by

$$\mathcal{T}_\gamma^{-1}(dx)|x\rangle = \left|\frac{x - dx}{1 + \gamma dx}\right\rangle. \quad (3)$$

Another relevant property is that $\mathcal{T}_\gamma$ becomes an identity operator when the infinitesimal translation goes to zero,

$$\lim_{dx\to 0} \mathcal{T}_\gamma(dx) = \mathbb{1}. \quad (4)$$

At this point we observe that, if we consider $\gamma = 1 - q$, the operator $\mathcal{T}_\gamma(x)$ is the infinitesimal generator of the group represented by the so-called q-exponential function originally defined as [14,15]

$$\exp_q(x) \equiv [1 + (1 - q)x]^{\frac{1}{1-q}}, \quad (5)$$

where $\exp_q(a)\exp_q(b) = \exp_q[a + b + (1 - q)ab]$ and $\exp_1(a) = \exp(a)$. The definition (5) represents a crucial ingredient in the mathematical formalism of the generalized Tsallis thermostatistics [16] and its several applications related with nonadditive physical systems [17–19]. Associating $\mathcal{T}_\gamma(dx)$ with the q exponential and expanding it to first order in dx leads to

$$\mathcal{T}_\gamma(dx) \equiv \mathbb{1} - \frac{i\hat{p}_\gamma dx}{\hbar}, \quad (6)$$

where $\hat{p}_\gamma$ is a generalized momentum operator and we are using the fact that momentum is a generator of translation. Now considering that

$$\hat{x}\mathcal{T}_\gamma(dx)|x\rangle = (x + dx + \gamma xdx)|x + dx + \gamma xdx\rangle \quad (7)$$

and $\mathcal{T}_\gamma(dx)\hat{x}|x\rangle = x|x + dx + \gamma xdx\rangle$, we obtain the commutation relation

$$[\hat{x},\mathcal{T}_\gamma(dx)]|x\rangle \simeq dx(1 + \gamma x)|x\rangle, \quad (8)$$

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where the error is in second order in dx. Then we get

$$[\hat{x},\hat{p}_\gamma] = i\hbar(1+\gamma x), \tag{9}$$

with the following uncertainty relation:

$$\Delta x \Delta p_\gamma \geqslant \frac{\hbar}{2}(1+\gamma\langle x\rangle), \tag{10}$$

which expresses the fact that the uncertainty in a measurement depends on γ as well as on the average position of the particle. It is worth mentioning that a similar commutation relation is used to describe the so-called "q-deformed quantum mechanics" [20].

Next, it is straightforward to obtain an expression for the modified momentum operator in the x basis using the definition (6)

$$\hat{p}_\gamma|\alpha\rangle = -i\hbar(1+\gamma x)\frac{d}{dx}|\alpha\rangle. \tag{11}$$

From (11) the modified momentum operator can be shortened to $\hat{p}_\gamma = -i\hbar D_\gamma$, with

$$D_\gamma \equiv (1+\gamma x)\frac{d}{dx} \tag{12}$$

being a deformed derivative in space. In the x representation, the corresponding time-dependent Schrödinger equation is

$$i\hbar\frac{\partial}{\partial t}\langle x|\alpha,t\rangle = \langle x|H|\alpha,t\rangle, \tag{13}$$

and if we consider the Hamiltonian operator to be $H = \hat{p}_\gamma^2/2m + V(x)$, we arrive at the following differential equation:

$$i\hbar\frac{\partial}{\partial t}\psi(x,t) = -\left(\frac{\hbar^2}{2m}\right)D_\gamma^2\psi(x,t) + V(x)\psi(x,t). \tag{14}$$

We now focus our attention on the case of a single spinless particle system. If the wave function $\psi(x,t)$ is normalized, it is possible to define a probability density $\rho(x,t) = |\psi(x,t)|^2$. Using Eq. (14) it is straightforward to derive a modified continuity equation,

$$\frac{\partial\rho}{\partial t} + D_\gamma J_\gamma = 0, \tag{15}$$

where the probability flux is given by

$$J_\gamma = \frac{\hbar(1+\gamma x)}{2mi}\left(\psi^*\frac{d\psi}{dx} - \psi\frac{d\psi^*}{dx}\right). \tag{16}$$

For standing waves in a null potential, the wave function $\phi(x)$ satisfying (14) obeys

$$-\frac{\hbar^2}{2m}D_\gamma^2\phi(x) = E\phi(x), \tag{17}$$

or

$$\frac{\hbar^2}{2m_e}\frac{d^2\phi(x)}{dx^2} + \frac{\hbar^2}{2}\frac{d}{dx}\left(\frac{1}{2m_e}\right)\frac{d\phi(x)}{dx} + E\phi(x) = 0, \tag{18}$$

with $m_e \equiv m/(1+\gamma x)^2$ being the particle's *effective mass*, in perfect analogy with problems involving a position-dependent mass particle in semiconductor heterostructures [11]. Here this particular expression for the effective mass arises naturally from the nonadditive translation operator. Equation (18) can then be rewritten in the form of the Cauchy-Euler equation [21],

$$u(x)^2\frac{d^2\phi(x)}{du^2} + au(x)\frac{d\phi(x)}{du} + b\phi(x) = 0, \tag{19}$$

with $u(x) = (1+\gamma x)$, $a = 1$, and $b = 2mE/(\hbar^2\gamma^2)$. The general solution for Eq. (19) is

$$\phi(x) = \exp\left[\pm i\frac{k}{\gamma}\ln(1+\gamma x)\right], \tag{20}$$

where k is a continuous variable regarding the particle's wave vector. Although the wave function for a free particle is not the usual plane wave, it is also not normalizable and gives a continuous energy spectra for the particle, $E = \frac{\hbar^2k^2}{2m}$, that is independent of γ. For this free particle, the probability flux J_γ is the same as an object moving at the classical velocity $\hbar k/m$.

If we now assume that the particle is confined to a one-dimensional infinite well of length L, the boundary conditions $\phi(0) = 0$ and $\phi(L) = 0$ lead to the wave function,

$$\phi_n(x) = \begin{cases} A_n \sin\left[\frac{k_n}{\gamma}\ln(1+\gamma x)\right], & 0 < x < L, \\ 0, & \text{otherwise}, \end{cases} \tag{21}$$

where the wave vector is now quantized,

$$k_n = \frac{n\pi\gamma}{\ln(1+\gamma L)}, \quad \text{with} \quad n = 1,2,3,4,\ldots. \tag{22}$$

The energy for a confined particle can then be written as

$$E_n = \frac{\hbar^2n^2\pi^2\gamma^2}{2m\ln^2(1+\gamma L)}, \tag{23}$$

where $\ln(1+\gamma L)/\gamma$ corresponds to an effective dilated/contracted well that approaches L as $\gamma \to 0$.

In Fig. 1 we show how the energy levels of a particle confined to an infinite well increase with n for different

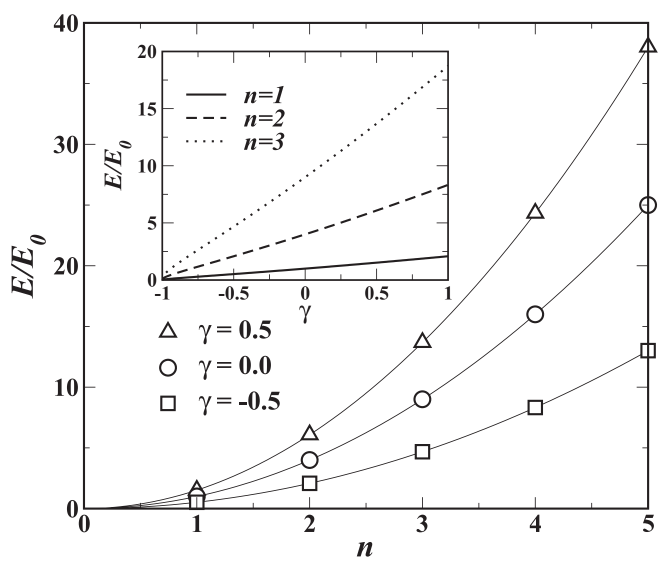

FIG. 1. The energy for a particle confined in an infinite well. The circles represent the energy for $\gamma = 0$, the squares $\gamma = -0.5$, and the triangles $\gamma = 0.5$. The energies are discrete; the solid lines are just guides for the eye. The inset shows the energy against γ for the three lowest levels.

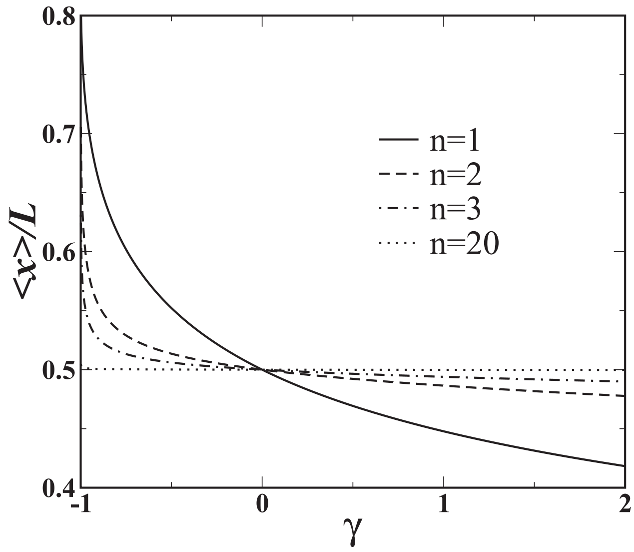

FIG. 2. The average position $\langle x\rangle$ of a particle confined in an infinite quantum well. The solid line gives the average value of x for $n=1$, the dashed line is for $n=2$, the case $n=3$ is the dashed-dotted line, and the large quantum number $n=20$ is represented by the dotted line. As n increases the asymmetry of the wave function is reduced, $\langle x\rangle \rightarrow 0.5$.

values of γ. Since the effective mass, m_e, in our description decreases with γ and since the lower the mass, the bigger is the kinetic energy of the particle, it means that the energy E_n increases with γ, as depicted in the inset of Fig. 1. The same reasoning can be applied to the size of the well; namely, the increase (decrease) of γ above (below) zero leads to a more pronounced contraction (dilation) of its effective length. The asymmetry caused by the parameter γ can be adequately quantified in terms of the average position of the particle in the box, calculated as $\langle x\rangle = \int_0^L \phi^* x \phi dx$. From (21), we obtain the expression

$$\langle x\rangle = \frac{L}{2}\left[\frac{\gamma^2+4k_n^2}{4(\gamma^2+k_n^2)} - \frac{3}{2}\frac{\gamma}{L(\gamma^2+k_n^2)}\right], \tag{24}$$

and the average of the modified momentum is $\langle p_\gamma\rangle = 0$. Figure 2 shows the average position of the particle against γ. As expected, when $\gamma = 0$ the average value is always 0.5. The ground state is the most affected by the nonadditivity of the space. As the quantum number increases, for example $n = 20$, the particle's average position becomes independent of γ, $\langle x\rangle \rightarrow 0.5$.

The position operator in other space directions still commutes. Therefore, the theory developed here can be easily extended for two and three dimensions. For example, when considering a square section of an infinite well, the corresponding wave function can be expressed as the product $\Phi(x,y) = \phi_1(x)\phi_2(y)$, where $\phi_1(x)$ and $\phi_2(y)$ are the wave functions in the x and y directions, respectively. The contour plots for the probability density $\rho(x,y)$ of a particle moving in a two-dimensional box are shown in Fig. 3(a) for $n_x = n_y = 1$, in Fig. 3(b) for $n_x = 1$, $n_y = 2$, in Fig. 3(c) for $n_x = n_y = 2$, and in Fig. 3(d) for $n_x = n_y = 20$, where we have used $\gamma = 1$ in all panels. The ground state shows clearly that the particle spends more time out of the box center. These results also indicate that the correspondence principle remains valid, as for $n_x = n_y = 20$ (large quantum numbers) the probability to find a particle is practically the same everywhere in the square well [see Fig. 3(d)].

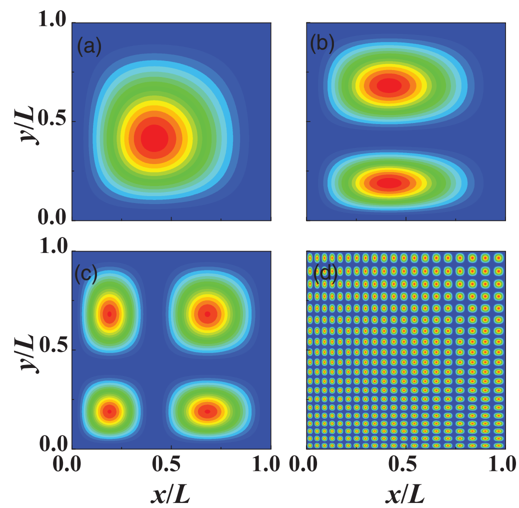

FIG. 3. (Color online) The contour plot of the probability density for a particle in a two-dimensional box for $\gamma = 1$, where the quantum numbers used are (a) $n_x = n_y = 1$, (b) $n_x = 1$, $n_y = 2$, (c) $n_x = n_y = 2$, and (d) $n_x = n_y = 20$. The probability increases from blue to red.

From the above examples, for a null (free particle) or a constant potential (infinite one-dimensional and two-dimensional well), the effect of γ on the wave function of the particle is to stretch or contract the space variable. In this way, we expect the same effect for a particle subjected to a potential barrier with height $V_0 > 0$, and located between $x = 0$ and $x = a$. The wave function becomes a linear combination of Eq. (20),

$$\phi(x) = \begin{cases} e^{ika'} + re^{-ika'}, & \text{for } x < 0, \\ Ae^{ik'a'} + Be^{-ik'a'}, & \text{for } 0 < x < a, \\ te^{ika'}, & \text{for } x > a, \end{cases} \tag{25}$$

where $k = \sqrt{2mE/\hbar^2}$, $k' = \sqrt{2m(E-V_0)/\hbar^2}$, and we used $a' = \ln(1+\gamma a)/\gamma$ for short. The coefficients A,B,r,t are found taking the continuity of the wave function and its spatial derivative in $x = 0$ and $x = a$. The transmission and tunneling probability is modified by γ

$$T^{-1} = |t|^2 = \begin{cases} 1 + \frac{V_0^2 \sin^2 k'a'}{4E(E-V_0)}, & \text{for } E > V_0, \\ 1 + \frac{V_0^2 \sinh^2 k'a'}{4E(V_0-E)}, & \text{for } E < V_0. \end{cases} \tag{26}$$

Figure 4 shows the transmission probability against the energy ratio E/V_0 for different values of γ. For $E > V_0$, we can see that the resonances ($T = 1$) depend on the value of γ. Increasing γ is analogous to decreasing the length of the barrier potential, and the transmission probability gets closer to 1. When $E < V_0$, the quantum tunneling probability increases with γ (thinner barrier). The inset in Fig. 4 shows an oscillation with increasing period for $E > V_0$.

Let us turn our attention to the kinetic operator developed through the nonadditive approach introduced here. According

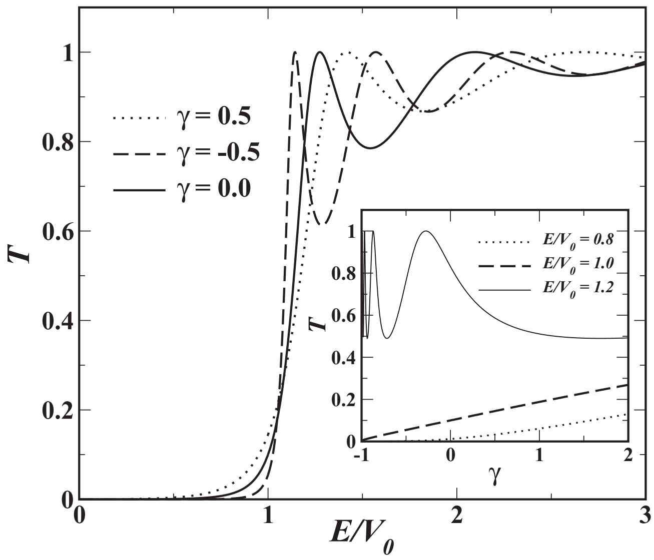

FIG. 4. The transmission probability T for a rectangular barrier for three different values of γ. The solid line is for the normal space ($\gamma = 0$). The dotted curve is for $\gamma = 0.5$, while $\gamma = -0.5$ corresponds to the dashed curve. The inset shows the transmission probability for three different values of energy. Here we used $\sqrt{2mV_0/\hbar^2} = 6$.

to Eq. (11), we can write the modified momentum operator as $\hat{p}_\gamma = (1 + \gamma x)\hat{p}$, so that the kinetic energy operator becomes

$$\hat{K} = \frac{1}{2}\frac{1}{\sqrt{m_e}}\hat{p}\frac{1}{\sqrt{m_e}}\hat{p}. \tag{27}$$

By comparison, this expression does not constitute a particular case of the general kinetic energy operator proposed in Ref. [22,23] to describe a position-dependent mass in the effective mass theory of semiconductors, namely, $\frac{1}{4}(m^\alpha \hat{p} m^\beta \hat{p} m^\delta + m^\delta \hat{p} m^\beta \hat{p} m^\alpha)$, with $\alpha + \beta + \delta = -1$. To the best of our knowledge, and despite its claimed generality in terms of the parameters α, β, and γ, this last operator has not been deduced from first-principles calculations.

In summary, we have introduced a nonadditive translation operator that can be identified as a q exponential [14,15]. By means of this operator, we have developed a modified momentum operator that naturally leads to a Schrödinger-like equation reminiscent of the wave equation typically used to describe a particle with position-dependent mass. First, our results indicate that a free particle in this formalism has a continuum energy spectrum with a wave function that is a modified plane wave. For a constant potential, like the problem of a particle confined to an infinite well, the energy now depends on the parameter γ, and for potential barrier, the peaks of maximum transmission probability are γ dependent. In this context, we can argue that the substrate, as defined here, behaves like a graded crystal whose local properties determine the effective mass of the confined particle. Our approach can therefore be useful to describe the particle's behavior within interface regions of semiconductor heterostructures. As future work, we intend to investigate the behavior of the nonadditive particle system when subjected to confining potentials that depend explicitly on position, for example, the harmonic oscillator or the central potential cases.

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