Revisiting the displacement operator for quantum systems with position-dependent mass

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Recently Costa Filho *et al.* [Phys. Rev. A **84**, 050102(R) (2011)] have introduced a position-dependent infinitesimal translation operator which corresponds to a position-dependent linear momentum and consequently to a quantum particle with position-dependent effective mass. Although there is no doubt about the novelty of the idea and the formalism, we believe that some aspects of the quantum mechanics in their original work could be enhanced. Here in this Brief Report first we address those points and then an alternative is introduced. Finally we apply the formalism for a quantum particle under a null potential confined in a square well, and the results are compared with those in the paper mentioned above.

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Particles with position-dependent mass in nonrelativistic quantum theory have attracted attention for the last few decades due to their application in nuclei, impurities in crystals, ^{3}He clusters, metal clusters, quantum liquids, semiconductor heterostructures, and so on [1]. Recently, using the generalized von Roos Hamiltonian together with the point canonical transformation, many attempts have been made to find exact solutions for quantum systems with position-dependent mass [2]. More recently, R. N. Costa Filho *et al.* [3] approached the problem in a different way. They introduced an infinitesimal translation operator in which a well-localized state around x can be transformed to another well-localized state around $x + (1 + \gamma x)\,dx$ i.e.,

$$\mathcal{T}_\gamma(dx)|x\rangle = |x + dx(1 + \gamma x)\rangle, \tag{1}$$

with all the other physical properties unchanged. Here, $\mathcal{T}_\gamma\,(dx)$ is the displacement operator, γ is a real constant with dimension (length)$^{-1}$, and dx is the infinitesimal change in the x coordinate. However, one should note that, from Ref. [3], since

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

and

$$\exp_q(a)\exp_q(b) = \exp_q[a + b + (1 - q)ab] \tag{3}$$

in which $\exp_q\,(a)$ is the q-exponential function, by rewriting $\gamma = \tilde{\gamma}\,(1 - q)$ where $\tilde{\gamma}$ has units of γ with value 1 and the Tsallis entropic index q is a real parameter, $\mathcal{T}_\gamma\left(dx'\right)$ can be considered as the infinitesimal generator of the group represented by the q-exponential function.

Using the standard form of the translation operator,

$$\mathcal{T}_\gamma\,(dx) = I - \frac{i\hat{p}_\gamma dx}{\hbar}, \tag{4}$$

it has been found in Ref. [3] that

$$\hat{p}_\gamma = -i\hbar(1 + \gamma x)\frac{d}{dx}, \tag{5}$$

in which $\hat{p}_\gamma$ is the generalized generator of the translation or the generalized linear momentum. It is easy to see that $\hat{p}_\gamma$ is not Hermitian, i.e., $\hat{p}_\gamma^\dagger \neq \hat{p}_\gamma$, which implies that $\mathcal{T}_\gamma\,(dx)$ is not unitary, $\mathcal{T}_\gamma\,(dx)^\dagger\,\mathcal{T}_\gamma\,(dx) \neq I$. Compared to the other conditions that $\mathcal{T}_\gamma\,(dx)$ may or may not fulfill, being unitary looks to be more reasonable. This is because the normalizability of the state ket remains invariant under the translation. By following the detailed calculation of Ref. [3], at first sight, it seems that we should sacrifice this condition for the new form of $\mathcal{T}_\gamma\,(dx)$, but by a simple manipulation this condition should not be forfeited. To see how, here we give an alternative form for $\hat{p}_\gamma$ which is Hermitian. Let us look at the details of finding the form of $\hat{p}_\gamma$. From (2) one writes

$$\begin{aligned}
&\left(I - \frac{i\hat{p}_\gamma\delta x}{\hbar}\right)|\alpha\rangle \\
&= \mathcal{T}_\gamma(dx)|\alpha\rangle = \int dx\mathcal{T}_\gamma(\delta x)|x\rangle\langle x|\alpha\rangle \\
&= \int dx|x + \delta x(1 + \gamma x)\rangle\langle x|\alpha\rangle \\
&= \int dx|x\rangle\langle x - \delta x(1 + \gamma x)|\alpha\rangle \\
&= \int dx|x\rangle\left(\langle x|\alpha\rangle - \delta x(1 + \gamma x)\frac{d\langle x|\alpha\rangle}{dx}\right) \\
&\simeq \int dx|x\rangle\left(\langle x|\alpha\rangle - \delta x(1 + \gamma x)\frac{d\langle x|\alpha\rangle}{dx}\right)|\alpha\rangle \\
&\quad + C\delta x\int dx|x\rangle\langle x|\alpha\rangle \\
&= \int dx|x\rangle\left(1 + C\delta x - \delta x(1 + \gamma x)\frac{d}{dx}\right)\langle x|\alpha\rangle,
\end{aligned} \tag{6}$$

in which C is a constant to be identified later. Here we should comment that the added term $C\,\langle x|\alpha\rangle\,\delta x$ in the limit $\delta x \to 0$ vanishes because $\psi_\alpha\,(x) = \langle x|\alpha\rangle$ is the wave function, which by definition is finite and square integrable. In other words, this term is negligible in comparison with the term $\langle x|\alpha\rangle$, so that $(1 + C\delta x)\,\langle x|\alpha\rangle \simeq \langle x|\alpha\rangle$.

Going back to Eq. (6), one finds a modified form of the generalized linear momentum operator as follows:

$$\hat{p}_\gamma = -i\hbar\left((1 + \gamma x)\frac{d}{dx} + C\right). \tag{7}$$

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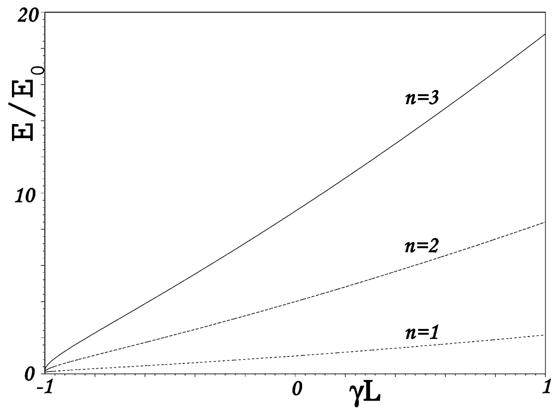

FIG. 1. Relative energy spectrum of a particle in an infinite square well and with effective mass (18) versus $\tilde{\gamma} = \gamma L$ for the three first states. In this figure E_0 is the ground-state energy of the particle in the limit $\gamma \to 0$, i.e., $E_0 = \pi^2\hbar^2/2mL^2$. The effect of γ is to increase ($\gamma > 0$) or decrease ($\gamma < 0$) the energy level.

To identify C we impose the Hermiticity condition for $\hat{p}_\gamma$, which yields

$$C = \frac{\gamma}{2}, \tag{8}$$

and therefore

$$\hat{p}_\gamma = -i\hbar\left((1+\gamma x)\frac{d}{dx} + \frac{\gamma}{2}\right). \tag{9}$$

It is reasonable that C vanishes when $\gamma \to 0$ because it guarantees that $\lim_{\gamma\to 0}\ \hat{p}_\gamma = -i\hbar\frac{d}{dx}$, which is expected. A unitary translation operator $\mathcal{T}_\gamma(dx)$ directly results from having $\hat{p}_\gamma$ Hermitian. To draw an analogy between our formalism and Ref. [3], we rewrite

$$\hat{p}_\gamma = -i\hbar D_\gamma, \tag{10}$$

where

$$D_\gamma = (1+\gamma x)\frac{d}{dx} + \frac{\gamma}{2} \tag{11}$$

is the modified derivative in this space. Following the standard quantum formalism for a particle with constant mass m under a real potential $V(x)$, one finds the Schrödinger equation

$$\hat{H}\psi_\alpha(x,t) = i\hbar\frac{\partial\psi_\alpha(x,t)}{\partial t}, \tag{12}$$

in which the Hamiltonian $\hat{H}$ reads

$$\hat{H} = \frac{\hat{p}_\gamma^2}{2m} + V(x). \tag{13}$$

We note here that unlike the case in Ref. [3] this Hamiltonian is Hermitian. For a particle of energy E and a null potential, the time-independent Schrödinger equation is given by

$$-\frac{\hbar^2}{2m}D_\gamma^2\phi(x) = E\phi(x), \tag{14}$$

which after some manipulation reads

$$u^2\phi''(u) + au\phi'(u) + b\phi(u) = 0. \tag{15}$$

Here $u = 1 + \gamma x$, $a = 3$,

$$b = \frac{2m}{\hbar^2\gamma^2}\tilde{E} = \frac{k^2}{\gamma^2}, \tag{16}$$

and

$$\tilde{E} = E + \frac{\hbar^2\gamma^2}{8m}. \tag{17}$$

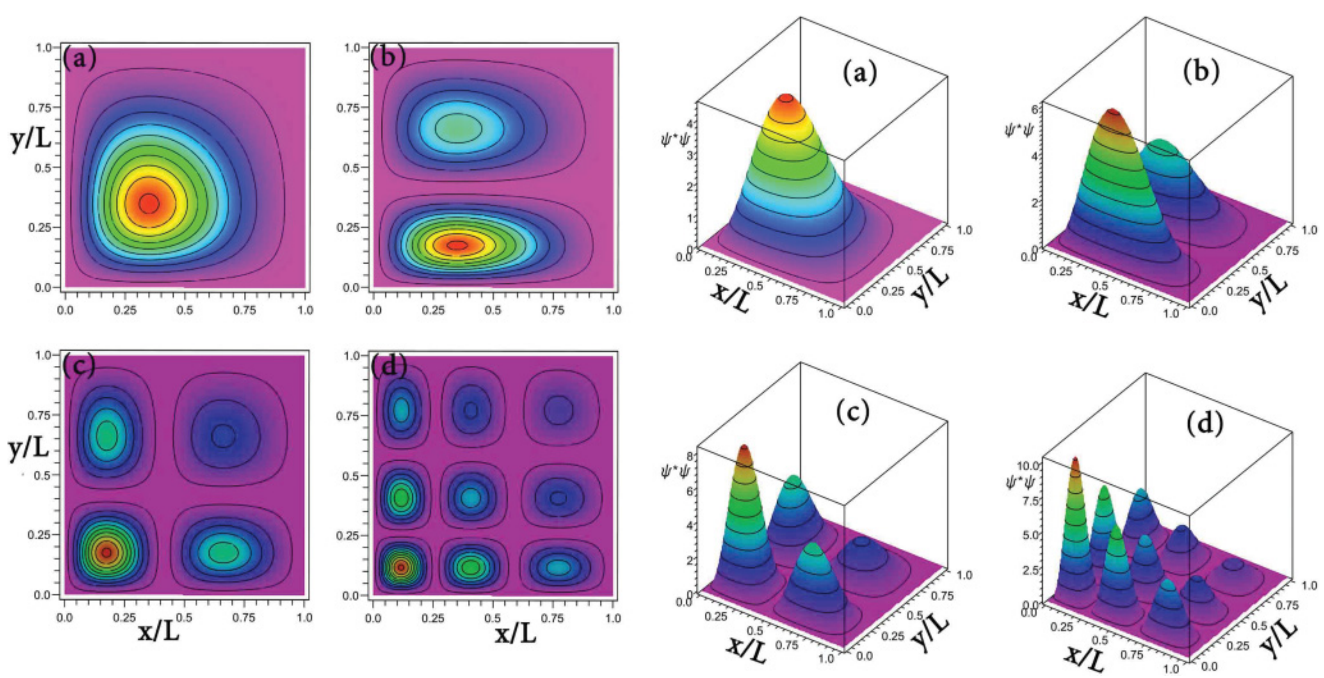

FIG. 2. (Color online) The probability density of a two-dimensional infinite square well for (a) $n_1 = 1, n_2 = 1$, (b) $n_1 = 1, n_2 = 2$, (c) $n_1 = 2, n_2 = 2$, and (d) $n_1 = 3, n_2 = 3$. Unlike the figure reported in [3], here the particle stays closer to the origin. In this figure the left side and the right side are the top and the side views, respectively, and the wave functions are normalized.

As in [3], (15) is equivalent to a particle with position-dependent mass with effective-mass function

$$m_e = \frac{m}{(1+\gamma x)^2}. \tag{18}$$

A general solution to (15) is given by

$$\phi(u) = \frac{1}{u}\exp\left(\pm i\sqrt{\frac{k^2}{\gamma^2}-1}\ln u\right) \tag{19}$$

in which to have a square-integrable function we set $\frac{k^2}{\gamma^2} - 1 > 0$, or equivalently

$$E > \frac{3\hbar^2\gamma^2}{8m}. \tag{20}$$

If we consider the particle inside an infinite well between $x = 0$ and $x = L$, the proper boundary conditions [i.e., $\phi(x=0) = 0 = \phi(x=L)$] would lead to the following wave function:

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

where

$$|A_n|^2 = \frac{2}{L} + 2\gamma + \frac{(1+\gamma L)}{2n^2\pi^2 L}\ln^2(1+\gamma L), \tag{22}$$

$$k_n^2 = \gamma^2\left(1 + \frac{n^2\pi^2}{\ln^2(1+\gamma L)}\right), \tag{23}$$

and finally the energy spectrum reads

$$E_n = \frac{n^2\pi^2\hbar^2\gamma^2}{2m\ln^2(1+\gamma L)} + \frac{3\hbar^2\gamma^2}{8m}. \tag{24}$$

One can easily show that in the limit $\gamma \to 0$ the above results will reproduce the usual infinite potential well for a particle with constant mass m. Here we would like to compare the effect of this configuration with those in Ref. [3]. As is clear, the form of the energy spectrum shows that the energy here is shifted up by the term $\frac{3\hbar^2\gamma^2}{8m}$ (see Fig. 1 for instance). Figure 2 displays the density function $|\psi|^2 = |\phi|^2$ of the two-dimensional infinite well for different values of the quantum numbers.

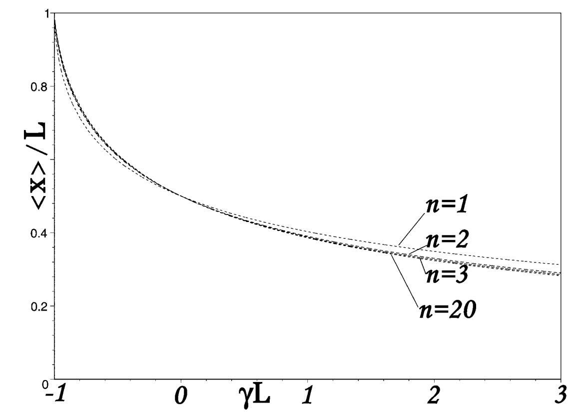

FIG. 3. $\langle x\rangle/L$ versus $\tilde{\gamma} = \gamma L$ of a one-dimensional particle in an infinite square well for $n = 1$, 2, 3, and 20. Although there are slight changes between the different cases, the general behaviors are almost the same, which is in contrast with the results of [3].

Following [3], we find the expectation value of the position of the particle in a one-dimensional infinite well, which is given by

$$\langle x\rangle = \int_0^L x|\phi_n(x)|^2 dx = \frac{(1+\gamma L)\ln(1+\gamma L)}{L\gamma^2} \times \left(1 + \frac{\ln^2(1+\gamma L)}{4\pi^2 n^2}\right) - \frac{1}{\gamma}. \tag{25}$$

This implies that $\lim_{\gamma\to 0}\langle x\rangle = \frac{L}{2}$. Figure 3 displays $\langle x\rangle/L$ versus $\tilde{\gamma} = \gamma L$ for different values of n. In contrast to [3], it is clear from Fig. 3 that n plays no significant role in the general behavior of the diagram. Also, after some manipulation one can show that the average of the modified momentum is zero, i.e., $\langle\hat{p}_\gamma\rangle = 0$, as was expected.

In conclusion, we add that our aim in this Brief Report is not to criticize the formalism given by the authors of Ref. [3] but instead to try to provide a different perspective on their new idea. Along this line we have shown how we could introduce a linear momentum operator which is Hermitian and at the same time matches with their formalism.

As a final point we note that, although the form of the Schrödinger equation found in Ref. [3] did not correspond with the generalized form of the kinetic energy operator proposed by von Roos [4], the counterpart equation (12) in this Brief Report is well consistent with the von Roos kinetic energy operator with the ordering parameters $\alpha = \gamma = \frac{-1}{4}$ and $\beta = \frac{-1}{2}$ [5].

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