Generalized space and linear momentum operators in quantum mechanics

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We propose a modification of a recently introduced generalized translation operator, by including a $q$-exponential factor, which implies in the definition of a Hermitian deformed linear momentum operator $\hat{p}_q$, and its canonically conjugate deformed position operator $\hat{x}_q$. A canonical transformation leads to a generator operator of spatial motion for the classical phase space may be expressed in terms of the generalized dual $q$-derivative. A position-dependent mass confined in an infinite square potential well is shown as an instance. Uncertainty and correspondence principles are analyzed.

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Systems consisting of particles with position-dependent mass (PDM) have been discussed by several researchers since few past decades. Applications of such systems may be found in semiconductor theory \cite{1}, $^4$He impurity in homogeneous liquid $^3$He \cite{2}, nonlinear optics \cite{3}, studies of inversion potential for NH$_3$ in density functional theory (DFT) \cite{4}, particle physics \cite{5}, and astrophysics \cite{6}.

Recently, Costa Filho et al. \cite{4,8} have introduced a generalized translation operator which produces infinitesimal displacements related to the $q$-algebra $\xi \mathbb{I} \mathbb{I}$, i.e.,

\[ \hat{T}_q(\varepsilon)|x\rangle \equiv |x + \varepsilon + \gamma\varepsilon x\rangle, \quad (1) \]

where $\gamma$ is a parameter with dimension of inverse length. This operator leads to a generator operator of spatial translations corresponding to a position-dependent linear momentum given by $\hat{p}_\gamma = (1 + \gamma\hat{x})\hat{p}$, and consequently a particle with position-dependent mass. This operator was used to solve problems of particles with position-dependent mass in the quantum formalism. This deformed momentum operator is not Hermitian, which led Mazharimousavi \cite{11} to introduce a modification in its definition. Other generalizations have been also appeared in the literature, particularly a nonlinear version of Schrödinger, Klein-Gordon, and Dirac equations \cite{12-14}.

We introduce a nonnormalized generalized phase factor in Eq. (1) as

\[ \hat{T}_q(\varepsilon)|x\rangle \equiv \exp_q \left[ \frac{ig(x)\varepsilon}{\hbar} \right] |x + \varepsilon + \frac{1 - q}{\xi} \varepsilon x\rangle \]
\[ = \exp_q \left[ \frac{ig(x)\varepsilon}{\hbar} \right] |\xi (\hat{x} \oplus_q \varepsilon)\rangle, \quad (2) \]

where $g(x)$ is a continuous function with dimension of linear momentum ($g(x) = 0$ recovers Eq. (1)), $\varepsilon$ is an infinitesimal displacement, the symbol $\oplus_q$ represents the $q$-addition operator, $a \oplus_q b = a + b + (1 - q)ab$ \cite{9,10}, $\xi$ is a characteristic length, $\tilde{x} \equiv x/\xi$ is the dimensionless position, and the dimensionless parameter $q$ controls the generalization of the exponential function $\exp_q x \equiv [1 + (1 - q)x]^1/(1 - q)$, with $|A|_+ \equiv \max\{A, 0\}$ \cite{11}. The symbol $\gamma$ in Eq. (1) (as it appears in \cite{8}) has been here changed to $\gamma_q \equiv (1 - q)/\xi$ once the $q$-addition shall be used with dimensionless variables.

The $q$-exponential of an imaginary number yields generalized trigonometric functions \cite{10}, and it can be written as $\exp_q(\pm ix) = \rho_q(x)\exp_q(\pm i\tilde{x})$, with $\rho_q(x) = \exp_q(ix)\exp_q(-ix) = \exp_q[(1 - q)x^2]$ ($x \in \mathbb{R}$); $\rho_q(x)$ is the norm of the $q$-exponential. $q = 1$ recovers the usual exponential function, and the $q$-exponential factor reduces to a usual phase factor with unitary norm. The $q$-exponential function satisfies

\[ \exp_q(a)\exp_q(b) = \exp_q(a \oplus_q b) \quad (3) \]

where $a$ and $b$ are two dimensionless quantities.

Similarly to the operator defined by Eq. (1), $\hat{T}_q(\varepsilon)$ also forms a group, i.e.,

\[ \hat{T}_q(\xi\hat{x}_1)\hat{T}_q(\xi\hat{x}_2)|0\rangle = \hat{T}_q(\xi(\hat{x}_1 \oplus_q \hat{x}_2))|0\rangle. \quad (4) \]

Application of the operator $\hat{T}_q(\varepsilon)$ on state $|0\rangle$, repeated $n$ times, leads to

\[ \hat{T}_q^n(\varepsilon)|0\rangle = \exp_q \left[ n \oplus_q \frac{ig(x)\varepsilon}{\hbar} \right] |n \oplus_q \varepsilon\rangle, \quad (5) \]

where $n \oplus_q x$ is a generalized product \cite{10}:

\[ n \oplus_q x = \frac{1}{1 - q} \left\{ [1 + (1 - q)x]^n - 1 \right\}. \quad (6) \]

(Not to confound the generalized product $n \oplus_q x$ with another generalization, frequently known as $q$-product,
If $\psi(x)$ is the generator of generalized infinitesimal translations. Expanding $T_q(\epsilon)$, and $\psi(x)$ (Eq. (3)), up to the first order in $\epsilon$, we get

$$T_q(\epsilon) = 1 - \frac{i\epsilon}{\hbar} \hat{p}_q + ...,$$

$$\psi(x) = (1 - \gamma \epsilon + ...)(1 + \epsilon A + ...) \times \left[ \psi(x) - \epsilon(1 + \gamma x) \frac{d\psi}{dx} + ... \right],$$

where $A$ is a constant taken from the expansion of $exp(q(x)\epsilon/\hbar)$ in powers of $\epsilon$, and we have

$$\langle x|\hat{p}_q|\psi \rangle = -i\hbar \frac{d}{dx}[(1 + \gamma q(x))\psi(x)] + i\hbar A\psi(x). \quad (15)$$

Imposition that $\hat{p}_q$ is Hermitian implies $A = \gamma q/2$, then

$$\hat{p}_q = \hat{p} \gamma \hat{x} + \hat{p} (1 + \gamma \hat{x}) = \frac{1}{2} i\hbar \gamma A \hat{p} \gamma \hat{x} - \frac{1}{2} i\hbar \gamma A \hat{p}, \quad (16)$$

i.e.,

$$\hat{p}_q = \frac{\hat{p} (\gamma \hat{x})}{2} + \hat{p} \gamma \hat{x}, \quad (17)$$

with $[\hat{x}, \hat{p}] = i\hbar \hat{1}$.

We introduce a generalized space operator $\hat{x}_q$ such that $[\hat{x}_q, \hat{p}_q] = i\hbar \hat{1}$. Recalling the property $[f(\hat{x}), \hat{p}] = i\hbar f'(\hat{x})$, with $\hat{x}_q = f(\hat{x})$, we arrive at

$$\hat{x}_q = \frac{\ln(1 + \gamma q \hat{x})}{\gamma q} = \xi \ln[exp(q(x)/\xi)]. \quad (18)$$

The transformation (18) is already appeared in a different context, as the real part of a transformation of a complex number $z$ into a kind of generalized complex number $\zeta = \exp z$, and this allows the $q$-Euler formula to be expressed as $exp_q z = exp_1 \zeta_q$. Even before that, the transformation (18) had also appeared connecting Tsallis (nonadditive) entropy with Rényi (additive) entropy [19].

According to Ehrenfest’s theorem, the time evolution of the expectation values of the space $\hat{x}$ and linear momentum $\hat{p}$ operators are given respectively by

$$\frac{d\langle \hat{x} \rangle}{dt} = \frac{\langle (1 + \gamma q \hat{x})^2 \rangle}{2m} + \langle \frac{\hat{p} (1 + \gamma q \hat{x})^2}{2m} \rangle, \quad (19a)$$

and

$$\frac{d\langle \hat{p} \rangle}{dt} = -\left( \frac{dV}{dx} \right) - \gamma_q \left( \gamma_q \hat{p} \gamma \hat{x}^2 \right) - \gamma_q \left( \hat{p}^2 (1 + \gamma q \hat{x}) \right), \quad (19b)$$

where we have used the following commutation relations:

$$[\hat{x}, \hat{p}_q^2] = i\hbar (1 + \gamma q \hat{x})^2 \hat{p} + i\hbar \hat{p} (1 + \gamma q \hat{x})^2, \quad (20)$$

and

$$[\hat{p}, \hat{p}_q^2] = -i\hbar \gamma_q (1 + \gamma q \hat{x}) \hat{p}^2 - i\hbar \gamma_q \hat{p}^2 (1 + \gamma q \hat{x}). \quad (21)$$

The operators $\hat{x}_q$ and $\hat{p}_q$ present the following classical analogs:

$$\hat{p}_q = (1 + \gamma q \hat{x}) \hat{p}, \quad (22a)$$

and

$$\hat{x}_q = \frac{\ln(1 + \gamma q \hat{x})}{\gamma q} = \xi \ln[exp(q(x)/\xi)]. \quad (22b)$$

$$d\langle \hat{x} \rangle = \int dx \psi^*(x) (x + \epsilon + \gamma q x) \psi(x) \frac{(1 - q) \epsilon^2 s(x)/\hbar^2}{1 + \gamma q \epsilon}, \quad (10)$$

The first order approximation in $\epsilon$ is represented by the $q$-addition:

$$\langle \hat{x} \rangle = \langle \hat{x} \rangle + \epsilon + \gamma q \langle \hat{x} \rangle \epsilon. \quad (11)$$
with \( \{x,q\}_{(x,p)} = 1 \). The generating function of the canonical transformations given by Eq.’s (22) is \( \Phi(x,q) = -p(x^2 - 1)/\gamma_q \).

As an application, let us address a constant mass particle and linear momentum \( p_q \) under the influence of a conservative force with potential \( V(x_q) \), whose Hamiltonian is

\[
K(x_q, p_q) = \frac{p_q^2}{2m} + V(x_q).
\]

The canonical transformations (22) lead to the new Hamiltonian (see, for instance, [20])

\[
H(x, p) = \frac{p^2}{2m(x)} + V(x),
\]

where the particle mass depends on the position \( x \) as

\[
m(x) = \frac{m}{(1 + \gamma_q x)^2}.
\]

The equation of motion is

\[
\ddot{\gamma}_q = \frac{m}{2} \gamma_q \dot{x}^2 - \frac{\gamma_q \dot{x}^2}{(1 + \gamma_q x)^3} = -\frac{dV(x)}{dx},
\]

with \( p = m(x)\dot{x} \), thus

\[
m \left[ \frac{\ddot{x}}{(1 + \gamma_q x)^2} - \frac{\gamma_q \dot{x}^2}{(1 + \gamma_q x)^3} \right] = -\frac{dV(x)}{dx}.
\]

This equation may be conveniently rewritten as

\[
m \dddot{x} + x(t) = F(x),
\]

i.e., a deformed Newton’s law for a space with non-linear displacements, where \( \dddot{x} = \frac{d^2}{du^2} \) is the second \( q \)-derivative, defined as \( \dddot{x} = \lim_{u \to a} \frac{f(u)-f(a)}{u-a} = \frac{1}{1+(1-q)f(u)/du} \). The second \( q \)-derivative must be taken as

\[
\dddot{x}_q = \frac{1}{1+(1-q)f(u)/du} \frac{d}{du} \left[ \frac{1}{1+(1-q)f(u)/du} \right] \frac{df}{du}.
\]

Similarly to what was done in the (different) generalized derivative introduced by [12].

The generalized displacement of a position-dependent mass in a usual space \((dx)\) is mapped into a constant mass in a deformed space with usual displacement \((dx_q)\): \( dx_q = \xi \left[ \frac{d}{dx} \right] \approx \frac{dx}{1 + \gamma_q x} \approx dx_q \). The temporal evolution is governed by the generalized dual derivative, \( \dddot{x_q} = \frac{1}{1+\gamma_q x} \frac{dx}{dt} \).

The probability \( P_{\text{class}} dx \propto dx/v \) to find a classical particle with position-dependent mass given by Eq. (25), between \( x \) and \( x + dx \), constrained to \( 0 \leq x \leq L \), and free of forces, is

\[
\frac{1}{(1 + \gamma_q x) \ln(1 + \gamma_q L)} dx.
\]

Note that the probability density \( P_{\text{classic}} \) is independent of the initial condition, and the uniform distribution \( P_{\text{classic}} \to 1/L \) is recovered as \( \gamma_q \to 0 \).

The first and second moments of the classical distribution according to position and momentum are

\[
\overline{p} = \frac{\gamma_q L - \ln(1 + \gamma_q L)}{\gamma_q \ln(1 + \gamma_q L)},
\]

\[
\overline{p^2} = \frac{\gamma_q^2 L^2 - 2\gamma_q L + 2 \ln(1 + \gamma_q L)}{2 \gamma_q \ln(1 + \gamma_q L)},
\]

\[
\overline{\overline{p}} = 0,
\]

and

\[
\frac{1}{2m} \overline{p^2} = mE \left[ \frac{(1 + \gamma_q L)^2 - 1}{2(1 + \gamma_q L)^2 \ln(1 + \gamma_q L)} \right],
\]

where \( \lim_{\gamma_q \to 0} \overline{p} = L/2 \), \( \lim_{\gamma_q \to 0} \overline{p^2} = L^2/3 \), \( \lim_{\gamma_q \to 0} \overline{\overline{p}} = 2mE \), and \( E \) is the energy of the particle.

Consider a system described by the Hamiltonian operator \( K \) at coordinate basis \( \{|x_q\} \). The time independent Schrödinger equation for a particle in a null potential at the basis \( \{|x_q\} \) is

\[
\frac{1}{2m} \frac{\overline{p^2}}{\psi} = E|\psi\rangle.
\]

Using Eq. (17), we have:

\[
-\frac{(1 + \gamma_q x)^2 h^2}{2m} \frac{d^2 \psi}{dx^2} - \frac{h^2 \gamma_q (1 + \gamma_q x)}{m} \frac{d\psi}{dx} - \frac{h^2 \gamma_q^2}{8m} \psi(x) = E \psi(x),
\]

which can be rewritten in the form

\[
u(x) \frac{d^2 \psi(u)/du^2 + au \frac{d\psi}{du} + b\psi(u) = 0,
\]

with \( u(x) = 1 + \gamma_q x, a = 2 \), and \( b = \frac{2m}{h^2} \left[ E + \frac{h^2 \gamma_q^2}{8m} \right] \).

Similarly to what was done in [7] and [11], Eq. (33) corresponds to a position-dependent mass particle according to Eq. (25). The solution of Eq. (33) is given by

\[
\frac{\psi(x)}{\sqrt{1 + \gamma_q x}} \exp \left[ \pm \frac{ik}{\gamma_q} \ln(1 + \gamma_q x) \right] = \frac{\psi_0}{\sqrt{1 + (1 - q)x/\xi}} \exp(x/\xi) \pm ik \xi
\]

and presents a singularity at \( x = -1/\gamma_q \).

For a particle inside an infinite square potential well between \( x = 0 \) and \( x = L \), the eigenfunctions and energies of the particle are respectively given by

\[
\psi_n(x) = \frac{A_{q,n}}{\sqrt{1 + \gamma_q x}} \sin \left[ \frac{k_{q,n} \gamma_q}{\gamma_q} \ln(1 + \gamma_q x) \right]
\]

(36)
for $0 \leq x \leq L$, and $\psi_n(x) = 0$ otherwise, and
\[ E_n = \frac{\hbar^2 \pi^2 \gamma_n^2 n^2}{2m \ln^2(1 + \gamma_n L)} \]  
(37)

with $A_{n,n}^2 = 2\gamma_n / \ln(1 + \gamma_n L)$, $k_{n,n} = n\pi\gamma_n / \ln(1 + \gamma_n L)$ ($n$ is a integer number). The wave function differs from those found in [7], and [11], though it is similar to that one obtained in [21]. Nevertheless, the energy levels are the same of those in [7].

Figure 1 shows the wave functions and their respective probability densities for the three states of lowest energy, and Figure 2 illustrates four instances of the probability density $P(x, y) = |\psi_{n_1}(x)\psi_{n_2}(y)|^2$ for the case of a particle with position-dependent mass in a bidimensional box. It can be seen an asymmetry introduced by the position-dependent mass — the probability to find the particle around $x = 0$ increases as $\gamma_n L$ increases.

These results reduce to the usual problem of a particle confined in an infinite square well in the limit $\gamma_n \to 0$. We can see from Figure 2 that the average value of the quantum probability density approaches the classical one for large quantum numbers (here exemplified with $n = 10$), consistent with the correspondence principle.

The expectation values of $\langle \hat{x} \rangle$, $\langle \hat{x}^2 \rangle$, $\langle \hat{p} \rangle$, and $\langle \hat{p}^2 \rangle$ for the particle in a one dimensional infinite well are given by
\[ \langle \hat{x} \rangle = \frac{\gamma_n L - \ln(1 + \gamma_n L)}{\gamma_n \ln(1 + \gamma_n L)} - \frac{L \ln(1 + \gamma_n L)}{\ln^2(1 + \gamma_n L) + (2n)^2}, \]  
(38a)
\[ \langle \hat{x}^2 \rangle = \frac{\gamma_n^2 L^2 - 2\gamma_n L + 2 \ln(1 + \gamma_n L)}{2\gamma_n^2 \ln(1 + \gamma_n L)} + \frac{1 - (1 + \gamma_n L)^2 \ln(1 + \gamma_n L)}{2\gamma_n^2 \ln^2(1 + \gamma_n L) + n^2 \pi^2} + \frac{2\gamma_n L \ln(1 + \gamma_n L)}{\gamma_n^2 \ln^2(1 + \gamma_n L) + 4n^2 \pi^2}, \]  
(38b)
\[ \langle \hat{p} \rangle = 0, \]  
(38c)
\[ \langle \hat{p}^2 \rangle = \frac{\hbar^2 [1 + \gamma_n L]^2 - 1}{2(1 + \gamma_n L) \ln(1 + \gamma_n L)} \frac{k_{n,n}^2}{k_{n,n}^2 + \gamma_n^2} \times \left[ (k_{n,n} - \frac{i\gamma_n}{2}) (k_{n,n} + \frac{i\gamma_n}{2}) + \frac{\gamma_n^2}{4} \right]. \]  
(38d)

Clearly we can see that in the limit $n \to \infty$, Eq.'s (38) coincide with Eq's (31), obtained by the analogous problem described in the classical formalism. Also easily one can show that the limit $\gamma_n \to 0$ recovers the usual results $\langle \hat{x} \rangle \to \frac{L}{2}$, $\langle \hat{x}^2 \rangle \to \frac{L^2}{4}$, and $\langle \hat{p}^2 \rangle \to \hbar^2 k_{n,n}^2$ with $E_n = \hbar^2 k_{n,n}^2 / 2m$ ($k_{n,n} \equiv k_{1,n} = 2\pi n / L$).

Since the operators $\hat{x}$ and $\hat{p}$ are Hermitian and canonically conjugated, the uncertainty relation is satisfied for

\[ \langle \hat{x} \rangle \langle \hat{p} \rangle \geq \frac{\hbar}{2}, \]  
(39)

Given the density $\rho_\| = |\psi_{n_1}(x)\psi_{n_2}(y)|^2$ for a particle confined in a bidimensional box within a generalized space with $\gamma_n L = 2$, and (a) $(n_1, n_2) = (1, 1)$, (b) $(n_1, n_2) = (1, 2)$, (c) $(n_1, n_2) = (2, 2)$, (d) $(n_1, n_2) = (3, 3)$. Color scale ranges from blue (low probabilities) to red (high probabilities).
different values of $\gamma_q$, *i.e.* $\langle(\Delta \hat{x})^2(\Delta \hat{p})^2\rangle \geq \hbar^2/4$ (see Figure 4). Note that the product $\langle(\Delta \hat{x})^2(\Delta \hat{p})^2\rangle$ is minimum for $\gamma_q = 0$.

Finally, we conclude that the modified generalized translation operator $\hat{T}_q(\varepsilon)$ (Eq. 2) preserves the properties of that one introduced by [7], Eq. (11). The corresponding generalized linear momentum operator $\hat{p}_q$, which is the generator of these translations, is Hermitian, as suggested by [11]. The canonical transformation $(\hat{x}, \hat{p}) \rightarrow (\hat{x}_q, \hat{p}_q)$ leads the Hamiltonian of a system with position-dependent mass given by $m(x) = m/(1 + \gamma_q x)^2$ to another one of a particle with constant mass. Hermiticity permits the existence of classical analogs of the operators. Particularly, the classical equation of motion in the phase space may be compactly rewritten with the second dual $q$-derivative. We have revisited the problem of a particle confined within an infinite square well, as discussed by [7], [11] and [21]. The results are consistent with the uncertainty and correspondence principles, as expected, once these dynamical variables are canonical and Hermitian.

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