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Exactly solvable model of the one-dimensional confined harmonic oscillator

Elchin I. Jafarov · Aynura M. Jafarova · Roy Oste

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Abstract. An exactly solvable model of the one-dimensional quantum harmonic oscillator confined in a box with infinite walls is constructed. We have found explicit expressions of the non-equidistant energy spectrum as well as stationary states wavefunctions in both momentum and position configuration spaces. It is shown that they are expressed through continuous q-Hermite polynomials. We have also found an explicit expression for the kernel of the finite-continuous Fourier transform between these two representation spaces.

Keywords. Confined quantum oscillator · Continuous q-Hermite polynomials · Finite-continuous Fourier transform

Mathematics Subject Classification (2010): 33D45 · 37N20 · 39A13

1 Introduction

Quantum mechanical systems being described within the confinement effect are very important because of their wide range of applications in nanostructures and condensed matter physics. The construction of models for such systems having explicit solutions is therefore especially valuable. It is well known that crystals having structures of the nanometer range, exhibit strong quantum confinement effects [10]. During fabrication of the artificial nanostructure, quantum confinement can be established in 1-, 2- or 3-dimensions. Depending on the number of free dimensions, quantum confined structures also change. If a bulk crystal has 3 free dimensions, then, quantum confinement towards one of them leads to so-called quantum well structures [5]. The mathematical description of such systems is based on the solution of the 1D Schrödinger equation with a certain external potential that acts on a finite interval. Unlike the case of unconfined harmonic oscillators, at present, there

E.I. Jafarov
Institute of Physics, Azerbaijan National Academy of Sciences, Javid av. 33, AZ-1143 Baku, Azerbaijan
E-mail: ejafarov@physics.ab.az

A.M. Jafarova
Institute of Mathematics and Mechanics, Azerbaijan National Academy of Sciences, B. Vahab-zade str. 9, AZ-1141 Baku, Azerbaijan
E-mail: aynura.jafarova@imm.az

Roy Oste
Department of Applied Mathematics, Computer Science and Statistics, Ghent University, Krijgslaan 281-S9, B-9000 Gent, Belgium
E-mail: Roy.Oste@UGent.be

is no unique approach for the construction of exactly-solvable quantum confined 1D oscillator models satisfying continuous orthogonality. The problem is that confinement imposed on the solution generally leads to approximate expressions for the energy spectrum and wavefunctions of its stationary states [1,4,11]. Also, there exists another approach in the case of the 1D quantum confinement, which is based on approximation of the confined harmonic oscillator problem by the well-known solutions in quantum mechanics for infinite quantum well or quantum box potentials [5]. Here, the question arises whether it is possible to solve this problem analytically? The existence of such a solution is very important, because, then, one will have expressions which are not approximations of the problem under consideration, but exact solutions of its generalization.

The aim of the current paper is to show one of the possible ways for the construction of an exactly-solvable quantum confined 1D harmonic oscillator model. Specifically, we will obtain explicit 1D solutions of the quantum mechanical oscillator problem on a finite-continuous interval.

Our paper is structured as follows: in section 2, we provide basic information about the stationary states of the non-relativistic one-dimensional quantum harmonic oscillator at canonical approach, whose position and momentum wavefunctions are expressed in terms of the Hermite polynomials. Moreover, we impose confinement on the definition of the harmonic oscillator potential which leads to the explicit solution of the problem under consideration in terms of the continuous q-Hermite polynomials. Further properties are discussed in section 3.

2 One-dimensional non-relativistic quantum harmonic oscillator at canonical approach and its explicit solution under confinement effect

Explicit solutions of one-dimensional non-relativistic quantum harmonic oscillator at canonical approach are well known. The explicit expressions of the wavefunctions in both position and momentum configuration representations are obtained as the exact solution of the 1D Schrödinger equation with the following Hamiltonian that acts on an infinite-continuous interval ($m = \omega = \hbar = 1$):

$$\hat{H}^{HO} = \frac{\hat{p}^2}{2} + \frac{\hat{x}^2}{2}. \tag{2.1}$$

Its stationary states in the x-representation are given in terms of Hermite polynomials [9]:

$$\psi_n^{HO}(x) = c_n e^{-x^2/2} H_n(x), \tag{2.2}$$

where, c_n is a normalization constant:

$$c_n = \frac{1}{\sqrt{2^n n! \sqrt{\pi}}},$$

and Hermite polynomials are defined in terms of ${}_2F_0$ hypergeometric functions as follows [8]:

$$H_n(x) = (2x)^n {}_2F_0 \left(\begin{array}{c} -n/2, -(n-1)/2 \\ - \end{array} ; -\frac{1}{x^2} \right).$$

As the wavefunctions (2.2) are orthonormalized, they satisfy the following orthogonality relation:

$$\int_{-\infty}^{\infty} \left[\psi_{n'}^{HO}(x)\right]^* \psi_n^{HO}(x) dx = \delta_{n',n}.$$

Stationary states of the one-dimensional non-relativistic quantum harmonic oscillator at canonical approach for the momentum p-representation can easily be obtained through the Fourier transform

$$\psi_n^{HO}(p) = \frac{1}{\sqrt{2\pi}} \int\limits_{-\infty}^{\infty} \psi_n^{HO}(x) e^{-ipx} dx,$$

where, $\psi_n^{HO}(p)$ is also expressed in terms of Hermite polynomials in the following manner:

$$\psi_n^{HO}(p) = (-i)^n c_n e^{-p^2/2} H_n(p). \tag{2.3}$$

The energy spectrum of the one-dimensional non-relativistic quantum harmonic oscillator at canonical approach is obtained as the eigenvalues of the Schrödinger equation

$$\hat{H}^{HO}\psi_n = E_n\psi_n,$$

and it has the following discrete-equidistant form:

$$E_n^{HO} = n + \tfrac{1}{2}, \quad n = 0, 1, 2, \ldots .$$

The dynamical symmetry of such an oscillator model is well known as the Heisenberg-Weyl algebra. Generators of this algebra are the creation a^+ and annihilation a^- operators, and the Hamiltonian $\hat{H}^{HO}$ itself. The creation and annihilation operators $a^\pm$ are defined as follows:

$$a^\pm = \frac{1}{\sqrt{2}} \left(\hat{x} \mp i\hat{p}\right).$$

It is also possible to re-express Hamiltonian (2.1) in terms of the creation and annihilation operators $a^\pm$ in the following manner:

$$\hat{H}^{HO} = \frac{1}{2} \left\{a^-, a^+\right\}.$$

Then, one observes that three generators of Heisenberg-Weyl algebra a^+, a^- and $\hat{H}^{HO}$ defined as shown above, satisfy the following commutation relations:

$$\left[a^-, a^+\right] = 1,$$
$$\left[\hat{H}^{HO}, a^\pm\right] = \pm a^\pm.$$

Expressing the momentum $\hat{p}$ and position $\hat{x}$ operators by means of the oscillator creation and annihilation operators $a^\pm$

$$\hat{p} = \frac{i}{\sqrt{2}} \left(a^+ - a^-\right), \tag{2.4}$$

$$\hat{x} = \frac{1}{\sqrt{2}} \left(a^+ + a^-\right), \tag{2.5}$$

one observes that the momentum and position operators satisfy the canonical commutation relation $[\hat{p}, \hat{x}] = -i$ and the three operators $\hat{p}$, $\hat{x}$ and Hamiltonian $\hat{H}^{HO}$ together satisfy the following Hamilton-Lie equations:

$$\left[\hat{H}^{HO}, \hat{p}\right] = i\hat{x},$$
$$\left[\hat{H}^{HO}, \hat{x}\right] = -i\hat{p}.$$

The model described above is accepted as the unconfined quantum harmonic oscillator model because all of the above relations are valid only if we work on the entire real line $(-\infty, +\infty)$. Now, the question arises whether it is possible to construct an exactly-solvable model of the one-dimensional quantum harmonic oscillator confined in a box with infinite walls:

$$V(x) = \begin{cases} x^2/2, & -a < x < a, \\ \infty, & \text{otherwise.} \end{cases} \tag{2.6}$$

However, solving the corresponding Schrödinger equation, where momentum and position operators satisfy the canonical commutation relation $[\hat{p}, \hat{x}] = -i$, does not lead to an explicit expression of the corresponding wavefunction, because the energy spectrum can only be computed numerically. One of the possible ways to find an explicit solution of the confined problem is to drop the canonical commutation relation ($[\hat{p}, \hat{x}] \neq -i$) and to define a new commutation relation, in the framework of which, one can obtain explicit expressions of the position and momentum wavefunctions, the corresponding Fourier transform for them and the energy spectrum of the model being constructed.

Before starting our approach for the construction of the one-dimensional quantum harmonic oscillator confined in a box with infinite walls, we provide some useful information regarding the continuous q-Hermite polynomials. They are one of the q-deformed analogues of the known Hermite polynomials and belong to the q-analogue of the Askey-scheme of hypergeometric orthogonal polynomials. The continuous q-Hermite polynomials are defined via ${}_2\varphi_0$ basic hypergeometric functions as follows [8]:

$$H_n(x|q) = e^{in\vartheta}\,{}_2\varphi_0\left(\begin{matrix} q^{-n}, 0 \\ - \end{matrix} \mid q; q^n e^{-2i\vartheta}\right), \; x = \cos\vartheta.$$

Unlike the regular Hermite polynomials, these polynomials satisfy an orthogonality relation that is finite and which holds for x from -1 to 1 as follows:

$$\frac{1}{2\pi}\int_{-1}^{1} \frac{w(x|q)}{\sqrt{1-x^2}} H_n(x|q)\, H_m(x|q)\, dx = \frac{\delta_{m,n}}{(q^{n+1};q)_\infty},$$

where,

$$w(x;a|q) = \left|\left(e^{2i\vartheta};q\right)_\infty\right|^2 = h(x,1)h(x,-1)h(x,q^{\frac{1}{2}})h(x,-q^{\frac{1}{2}}),$$

with

$$h(x,a) = \prod_{k=0}^{\infty}\left[1 - 2axq^k + a^2q^{2k}\right] = \left(ae^{i\vartheta}, ae^{-i\vartheta};q\right)_\infty, \quad x = \cos\vartheta.$$

Also, they satisfy the following three-term recurrence relation:

$$2xH_n(x|q) = H_{n+1}(x|q) + (1-q^n)\, H_{n-1}(x|q).$$

Since the following limit relation is known between the continuous q-Hermite and ordinary Hermite polynomials:

$$\lim_{q\uparrow 1} \frac{H_n\left(x\left(\frac{1-q}{2}\right)^{\frac{1}{2}} |q\right)}{\left(\frac{1-q}{2}\right)^{\frac{n}{2}}} = H_n(x),$$

one can apply the substitution $x \to x\sqrt{\frac{1}{2}(1-q)}$, which changes slightly both orthogonality and three-term recurrence relations as follows:

$$\frac{\sqrt{1-q}}{2\pi}\int\limits_{-\sqrt{\frac{2}{1-q}}}^{\sqrt{\frac{2}{1-q}}}\frac{w\left(x\sqrt{\frac{1}{2}(1-q)}|q\right)}{\sqrt{2-(1-q)x^2}}H_n\left(x\sqrt{\frac{1}{2}(1-q)}|q\right)$$

$$\times H_m\left(x\sqrt{\frac{1}{2}(1-q)}|q\right)dx=\frac{\delta_{m,n}}{(q^{n+1};q)_\infty},$$

$$\sqrt{2(1-q)}\cdot xH_n\left(x\sqrt{\frac{1}{2}(1-q)}|q\right)$$

$$=H_{n+1}\left(x\sqrt{\frac{1}{2}(1-q)}|q\right)+(1-q^n)\,H_{n-1}\left(x\sqrt{\frac{1}{2}(1-q)}|q\right).$$

Introducing orthonormal analogues of the continuous q-Hermite polynomials, we now have:

$$x\cdot\tilde{H}_n\left(x\sqrt{\frac{1}{2}(1-q)}|q\right)=\sqrt{\frac{d_{n+1}}{2(1-q)d_n}}\tilde{H}_{n+1}\left(x\sqrt{\frac{1}{2}(1-q)}|q\right)$$

$$+(1-q^n)\sqrt{\frac{d_{n-1}}{2(1-q)d_n}}\tilde{H}_{n-1}\left(x\sqrt{\frac{1}{2}(1-q)}|q\right),$$

where,

$$d_n=\frac{1}{(q^{n+1};q)_\infty}.$$

Then, simple computations show that

$$x\cdot\tilde{H}_n\left(x\sqrt{\frac{1}{2}(1-q)}|q\right)$$

$$=\frac{1}{\sqrt{2}}\left[\sqrt{[n+1]}\cdot\tilde{H}_{n+1}\left(x\sqrt{\frac{1}{2}(1-q)}|q\right)+\sqrt{[n]}\cdot\tilde{H}_{n-1}\left(x\sqrt{\frac{1}{2}(1-q)}|q\right)\right],$$

where,

$$[n]\equiv\frac{1-q^n}{1-q}.$$

For the realization of the q-Heisenberg-Weyl algbra, if we use the following definition of the position operator $\hat{x}$ that is similar to (2.5):

$$\hat{x}=\frac{1}{\sqrt{2}}\left(b^++b^-\right),$$

then, one observes the following action of the q-creation and annihilation operators to the basis vector:

$$b^+\left|n\right\rangle=\sqrt{[n+1]}\left|n+1\right\rangle,$$
$$b^-\left|n\right\rangle=\sqrt{[n]}\left|n-1\right\rangle.$$

As a consequence of such an action, the following q-deformation of the Heisenberg-Weyl algebra holds: b^{+} and b^{-} are first two generators of the deformed algebra. The definition of the third generator $\hat{N}$ is the following:

$$\hat{N}\left|n\right\rangle = [n]\left|n\right\rangle .$$

Finally, we have the following commutation relations for these generators:

$$\begin{aligned} \left[b^{\mp}, b^{\pm}\right]_{q^{\pm 1}} &= b^{\mp}b^{\pm} - q^{\pm 1}b^{\pm}b^{\mp} = [\pm 1]\,, \\ \left[\hat{N}, b^{\pm}\right]_{q^{\pm 1}} &= [\pm 1]\, b^{\pm}. \end{aligned}$$

Using all these new definitions, one can easily find the wavefunction of the stationary states in $\hat{x}$-representation for the one-dimensional quantum harmonic oscillator confined in a box with infinite walls (in case, when $a \equiv \sqrt{\frac{2}{1-q}}$). It has the following explicit form:

$$\tilde{\psi}_n^{cHO}\left(x\right) = \frac{\left(1-q\right)^{\frac{1}{4}}}{2^{\frac{1}{4}}\sqrt{2\pi}} \frac{\sqrt{\left(q^{n+1};q\right)_{\infty} w\left(\tilde{x}|q\right)}}{\left(1-\tilde{x}^2\right)^{\frac{1}{4}}} H_n\left(\tilde{x}|q\right). \tag{2.7}$$

Then, considering the momentum operator

$$\hat{p} = \frac{i}{\sqrt{2}}\left(b^{+} - b^{-}\right)$$

one has the following expression of the wavefunction in the p-representation:

$$\tilde{\psi}_n^{cHO}\left(p\right) = \frac{\left(-i\right)^n\left(1-q\right)^{\frac{1}{4}}}{2^{\frac{1}{4}}\sqrt{2\pi}} \frac{\sqrt{\left(q^{n+1};q\right)_{\infty} w\left(\tilde{p}|q\right)}}{\left(1-\tilde{p}^2\right)^{\frac{1}{4}}} H_n\left(\tilde{p}|q\right)$$

where

$$\tilde{x} = x\cdot\sqrt{\tfrac{1}{2}\left(1-q\right)}, \quad \tilde{p} = p\cdot\sqrt{\tfrac{1}{2}\left(1-q\right)}.$$

If we assume that the Hamiltonian is the same as in the undeformed quantum oscillator case:

$$\hat{H}^{cHO} = \frac{1}{2}\left(\hat{p}^2 + \hat{x}^2\right)$$

then the energy spectrum can be found from the action of the Hamiltonian on the wavefunction:

$$E_n^{cHO} = \frac{\left([n]+[n+1]\right)}{2} = \frac{1+q}{2}[n] + \frac{1}{2} \tag{2.8}$$

The new commutation relation between the momentum and position operators then has the following form:

$$[\hat{p},\hat{x}] = -i\frac{2}{[2]}[1-(1-q)\hat{H}^{cHO}].$$

One easily observes that it generalizes the known canonical commutation relation $[\hat{p},\hat{x}] = -i$ and under $q\to 1$ one completely recovers it. Because of this relation, one can write down the following generalizations of the Heisenberg equations:

$$\left[\hat{H}^{cHO},\hat{p}\right] = i\frac{2}{[2]}\hat{x} - i\frac{1-q}{1+q}\left\{\hat{x},\hat{H}^{cHO}\right\},$$

$$\left[\hat{H}^{cHO},\hat{x}\right]=-i\frac{2}{[2]}\hat{p}+i\frac{1-q}{1+q}\left\{\hat{p},\hat{H}^{cHO}\right\}.$$

As a consequence of all these definitions, one can introduce also the analogue of the Fourier transform, which is the following:

$$\tilde{\psi}_n^{cHO}(p)=\int\limits_{-\sqrt{2/(1-q)}}^{\sqrt{2/(1-q)}}K^{cHO}(x,p)\cdot\tilde{\psi}_n^{cHO}(x)\,dx,$$

where, the kernel of the confined Fourier transform $K^{cHO}(x,p)$ has the following explicit form:

$$K^{cHO}(x,p)=\sum_{n=0}^{\infty}\tilde{\psi}_n^{cHO}(p)\cdot[\tilde{\psi}_n^{cHO}]^*(x).$$

Substitution of the expressions for the wavefunctions in this series gives the following:

$$K^{cHO}(x,p)=\frac{1}{2\pi}\sqrt{\frac{1-q}{2}}\,(q;q)_\infty\,\frac{\sqrt{w(\tilde{x}|q)\,w(\tilde{p}|q)}}{\left[\left(1-\tilde{x}^2\right)\left(1-\tilde{p}^2\right)\right]^{\frac{1}{4}}}\sum_{n=0}^{\infty}(-i)^n\,\frac{H_n(\tilde{x}|q)\cdot H_n(\tilde{p}|q)}{(q;q)_n}.$$

To compute this, we use the following bilinear generating function for the continuous q-Hermite polynomials [3]:

$$\sum_{n=0}^{\infty}r^n\frac{H_n(\cos\theta|q)\cdot H_n(\cos\varphi|q)}{(q;q)_n}=\frac{\left(r^2;q\right)_\infty}{\left|\left(r\cdot e^{i(\theta+\varphi)};q\right)_\infty\left(r\cdot e^{i(\theta-\varphi)};q\right)_\infty\right|^2}.$$

We then have the following expression for the kernel of the Fourier transform:

$$K^{cHO}=\frac{1}{2\pi}\frac{\sqrt{\frac{1-q}{2}}\,(q;q)_\infty\,(-1;q)_\infty}{\left[\left(1-\tilde{x}^2\right)\left(1-\tilde{p}^2\right)\right]^{\frac{1}{4}}}$$

$$\times\frac{\sqrt{\left|\left(\left(\tilde{x}+\sqrt{\tilde{x}^2-1}\right)^2,\left(\tilde{p}+\sqrt{\tilde{p}^2-1}\right)^2;q\right)_\infty\right|^2}}{\left|\left(-i\left(\tilde{x}+\sqrt{\tilde{x}^2-1}\right)\left(\tilde{p}+\sqrt{\tilde{p}^2-1}\right),-i\frac{\tilde{x}+\sqrt{\tilde{x}^2-1}}{\tilde{p}+\sqrt{\tilde{p}^2-1}};q\right)_\infty\right|^2}.$$

One needs to note that all expressions introduced here reduce to their analogues for the one-dimensional oscillator without any confinement, when $a\to+\infty$ (this case is equivalent to limit case $q\to1$ where the q-Hermite polynomials reduce to the regular Hermite polynomials).

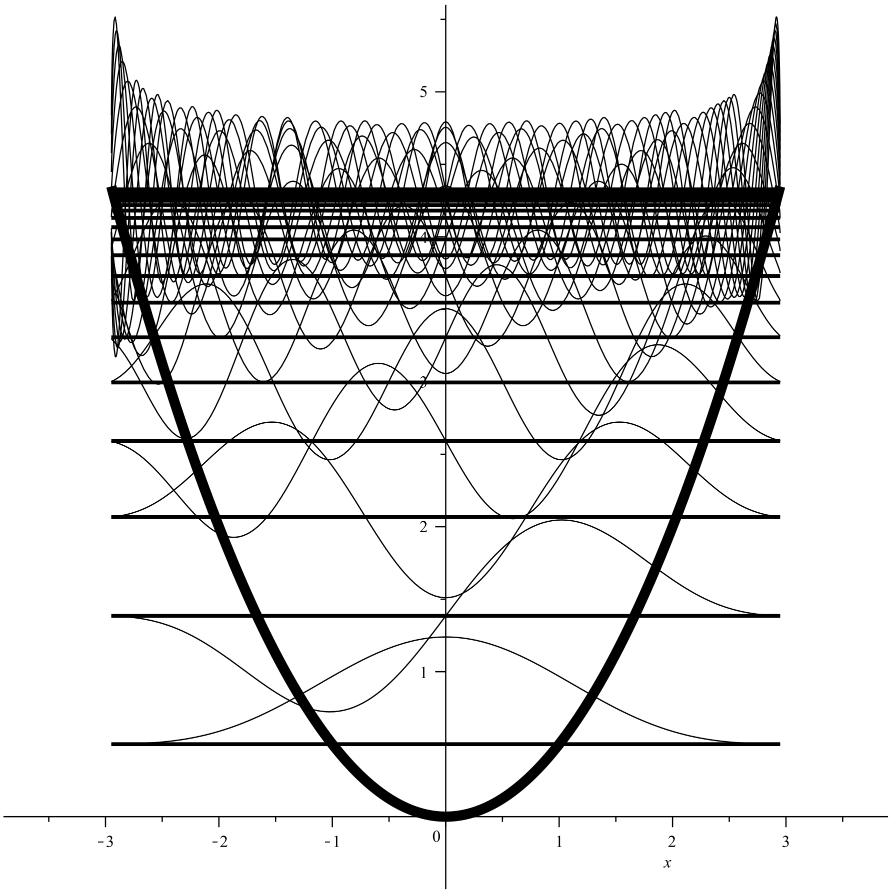

Fig. 1 Comparative plot of the confined potential (2.6), the wavefunctions (2.7) and the corresponding energy spectrum (2.8). The number of stationary states are chosen as $n = 0, 1, 2, \ldots, 20$. The free parameter q equals 0.77 which corresponds to a wall border parameter $a \approx 2.95$.

3 Discussions

In this paper, we constructed an exactly solvable model of the one-dimensional quantum harmonic oscillator confined in a box with infinite walls. Such a model has a number of applications in condensed matter physics, because by using it one can describe so-called quantum well structures or $GaAs/AlGaAs$ heterostructures. The advantage of our model is that it is exactly solvable. We managed to find explicit expressions for the energy spectrum, the wavefunctions in both momentum and position configuration spaces as well as a finite-continuous analogue of the Fourier transform between these two configuration spaces. It is shown that both wavefunctions of the stationary states are expressed in terms of the continuous q-Hermite polynomials. The energy spectrum which was written down in this paper, differs from its unconfined non-relativistic analogue in the sense that, in general, it is not equidistant. This can be observed visually also from the plot that is presented here. The plot is drawn for the case where q equals 0.77, which corresponds to a wall border parameter $a \approx 2.95$. As was mentioned at the end of the previous section, all these expressions reduce to the unconfined case, when $a \to +\infty$, which holds for limit $q \to 1$). For all other values, one observes that there is an overlap of ground state of both confined and unconfined models. Also, one needs to note that the 'distance' between the excited states is inversely related with the confinement size. Therefore, for values of q less than 1 there is almost overlap of the higher excited states. In our plot, we observe that almost half of the 20 excited states overlap with each other for case $n > 11$.

In this paper, we did not compute the limits mathematically, however, we note that we already did similar computations for Al Salam-Chihara polynomials in [2, 6, 7] and the same approach can be applied here to recover the unconfined expressions of the one-dimensional quantum harmonic oscillator.

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