PRAMANA
— journal of
physics

© Printed in India

Vol. 45, No. 4,
October 1995
pp. 311–317

The particle in a box problem in q-quantum mechanics

G VINOD, K BABU JOSEPH and K M VALSAMMA
Department of Physics, Cochin University of Science and Technology, Kochi 682 022, India

MS received 23 February 1995; revised 20 July 1995

Abstract. A q-deformed, q-Hermitian kinetic energy operator is realised and hence a q-Schrödinger equation (q-SE) is obtained. The q-SE for a particle confined in an infinite potential box is solved and the energy spectrum is found to have an upper bound.

Keywords. q-calculus; q-quantum mechanics; particle in a box.

PACS Nos 01·55; 02·90; 03·65

1. Introduction

The study of q-deformations of Lie algebras and ordinary calculus has grown into a major area of research in mathematical physics. The q-deformed calculus, when applied to quantum mechanics with its fundamental postulates preserved, gives rise to q-quantum mechanics. Several years ago Janussis *et al* [1, 2] discussed q-quantization and the eigenvalue problem of q-differential operators. Quantum mechanics is usually deformed in two different ways: one may either replace the canonical commutation relation by a q-commutation relation or the momentum operator in the Schrödinger equation (SE) by a q-deformed one. Most of the work in this area is based on the former approach [3–5]. Minahan [6] has considered a q-extension of SE (q-SE) and obtained the spectrum of q-harmonic oscillator. The energy spectrum of a q-analog of hydrogen atom has been obtained by Yang and Xu [7]. In this paper, following the q-SE method, we determine the spectrum of a particle in a one dimensional infinite potential well.

The infinite potential well is characterized by a constant potential in a finite region outside which the potential is infinite. Particles subject to such a potential are trapped inside the constant potential region. This model potential has been used in the free electron model of metals. Study of any problem in q-quantum mechanics is of interest not only for pedagogic reasons but also for comprehending the uniqueness of standard ($q = 1$) quantum mechanics. One cannot also rule out the possible existence of q-systems in nature.

2. Elements of q-calculus

The mathematical idea of q-deformation has deep roots running down to the middle of the last century. Further developments were achieved mainly due to the works of Jackson, Slater, Andrews and others [8]. A q-basic number is defined as

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

As $q \to 1, [n] \to n$. The q-factorial is

$$[n]! = [n][n-1][n-2]\ldots[2][1]. \tag{2}$$

The q-difference operator D_x is defined by

$$D_x f(x) = \frac{f(qx) - f(x)}{x(q-1)}. \tag{3}$$

If $q \to 1$, then the ordinary derivative d$f(x)$/d**x** is obtained, if it exists. The product rule and quotient rule for q-difference operators are

$$D_x\{u(x)v(x)\} = \{v(x)D_x u(x) + u(qx)D_x v(x)\} \tag{4}$$

$$D_x\{u(x)/v(x)\} = \frac{v(x)D_x u(x) - u(x)D_x v(x)}{v(qx)v(x)}. \tag{5}$$

The q-analogue of integration in the case of finite limits a, b is defined as:

$$S_a^b f(x) d(qx) = (1-q)\left\{b \sum_{r=0}^{\infty} q^r \phi(q^r b) - a \sum_{r=0}^{\infty} q^r \phi(q^r a)\right\}. \tag{6}$$

The product rule for q-integration is

$$Sv(x)D_x u(x)d(qx) = u(x)v(x) - Su(qx)D_x v(x)d(qx). \tag{7}$$

The q-analogues of exponential function and trigonometric functions have also been constructed

$$E_q(x) = \sum_{n=0}^{\infty} \frac{x^n}{[n]!} \tag{8}$$

$$\sin_q x = \frac{1}{2i}\{E_q(ix) - E_q(-ix)\} \tag{9}$$

$$\cos_q x = \frac{1}{2}\{E_q(ix) + E_q(-ix)\}. \tag{10}$$

3. *q*-quantum mechanics

Even though it is customary [8] to take the q-commutation relation

$$D_x x - qxD_x = 1$$

as the starting point of q-quantum mechanics, the D_x operator is neither q-Hermitian nor q-skew Hermitian (Appendix 1). Therefore it is not possible to define a simple and straightforward realisation of the momentum operator which is q-Hermitian. However this difficulty can be circumvented in an approach based on the q-Schrödinger equation which is written as

$$H_q \psi_q = E_q \psi_q \tag{11}$$

where the q-deformed Hamiltonian $\mathbf{H}_q$ is the sum of a q-deformed kinetic energy operator and a potential energy operator. Since in one dimension the kinetic energy operator contains d^2/dx^2 in the undeformed ($q = 1$) SE, we expect the q-deformed kinetic energy operator to contain $\mathbf{D}_x^2$. Besides, we demand that H_q is a q-Hermitian operator (Appendix 1). The q-adjoint operation is defined as

$$S\phi_q^*(x)\mathbf{A}\psi_q(x)d(qx) = S(\mathbf{A}^{\zeta}\phi_q(x))^*\psi_q(x)d(qx) \tag{12}$$

where the q-integration is over the q-line segment. Using (12) we can prove that

$$(\mathbf{D}_x)^{\zeta} = -\mathbf{D}_x\mathbf{q}^{-x\partial_x} \tag{13}$$

where the action of $q^{x\partial_x}$ is given by

$$q^{\pm x\partial_x}f(x) = f(q^{\pm 1}x)$$

So $\mathbf{D}_x^2\mathbf{q}^{-x\partial_x}$ serves as a q-hermitian operator (Appendix 1). We rewrite the q-SE as

$$\left\{\frac{-\hbar^2}{2m}\mathbf{D}_x^2\mathbf{q}^{-x\partial_x} + \mathbf{V}(\mathbf{x})\right\}\psi_q(x) = E_q\psi_q(x) \tag{14}$$

where E_q is a q-deformed energy eigenvalue.

In q-deformed space we can take $d(q\mathbf{x})$ as the elementary volume, or in the one dimensional problem $d(q\mathbf{x})$ serves as the elementary length. So $|\psi_q(x)|^2$ is the probability that a measurement performed on the system will locate it in the element $d(q\mathbf{x})$ of the q-line. Therefore, if we q-integrate $|\psi_q(x)|^2$ over the q-line segment of finite length, we will get unity

$$S|\psi_q(x)|^2 d(qx) = 1. \tag{15}$$

This probability interpretation demands $\psi_q(x)$ to be single valued and finite everywhere, as in the standard case. Also $\psi_q(x)$ and $D_x\psi_q(x)$ should vanish at endpoints of the q-line segment.

4. The particle in a box

In this problem,

$$V(x) = 0 \text{ for } 0 \leqslant x \leqslant a,$$
$$= \infty \text{ otherwise.} \tag{16}$$

We can write the q-SE for this potential as

$$(\mathbf{D}_x^2\mathbf{q}^{-x\partial_x} + k_q^2)\psi_q(x) = 0 \tag{17}$$

where

$$k_q^2 = \frac{2mE}{\hbar^2}. \tag{18}$$

Solution of the q-SE is

$$\psi_q(x) = N\sum_{r=0}^{\infty}\frac{(-1)^r q^{r(r+2)}(k_q x)^{2r+1}}{[2r+1]!} \tag{19}$$

N is the normalization constant. Since $\psi_q(0) = \psi_q(a) = 0$, the admissible solutions of $k_q a$ are those which satisfy

$$\sum_{r=0}^{\infty} \frac{(-1)^r q^{r(r+2)}(k_q a)^{2r+1}}{[2r+1]!} = 0. \tag{20}$$

Only numerical solutions of this equation are possible. From (18), the energy eigenvalues are given by

$$E_q = \frac{\hbar^2 (k_q a)^2}{2ma^2}. \tag{21}$$

The q-normalization constant N is evaluated from

$$S_{-\infty}^{\infty} \psi_q^*(x)\psi_q(x) d(qx) = 1 \tag{22}$$

which follows from the assumption that the particle is confined between $\mathbf{x} = 0$ and $\mathbf{x} = \mathbf{a}$. Let $\psi_q^* \psi_q$ be expressed as

$$\psi_q^*(x)\psi_q(x) = \sum_{r=0}^{\infty} b_r (k_q r)^{2r} \tag{23}$$

for even values of r,

$$b_r = -2 \sum_{s=0}^{(r-2)/2} \frac{q^{(r-s-1)(r-s+1)+s(s+2)}}{[2s+1]![2r-2s-1]!}$$

and for odd values of r,

$$b_r = 2 \sum_{s=0}^{(r-1)/2} \frac{q^{(r-s-1)(r-s+1)+s(s+2)}}{[2s+1]![2r-2s+1]!} - \frac{q^{(r-1)(r+3)/2}}{[r]![r]!}.$$

Since the series expansion of $\psi_q^*(kx)\psi_q(kx)$ is convergent, we may q-integrate each term in the expansion (24) employing the identity

$$S x^n d(qx) = \frac{x^{n+1}}{[n+1]} \tag{24}$$

which gives

$$N^2 \sum_{r=0}^{\infty} b_r \frac{k_q^{2r} a^{2r+1}}{[2r+1]} = 1$$

or,

$$N = \left\{ a \sum_{r=0}^{\infty} \frac{b_r (C_n)^{2r}}{[2r+1]} \right\}^{-1/2} \tag{25}$$

where C_n are the solutions of ka given by (20).

5. Analytic solutions for $q \approx 1$

Analytic solutions exist when q is close to unity. Let us take $q = 1 - \delta$, δ being a very small quantity. The following approximations are valid

$$[n] = n\{1 - (n-1)\delta/2\} \tag{26}$$

$$[n]! = n!\{1 - n(n-1)\delta/2\}. \tag{27}$$

The wavefunction is approximated by

$$\psi_q(kx) = N \sin_q k_q x + N \sum_{r=0}^{\infty} \frac{(-1)^{r+1}(kx)^{2r+1}}{(2r+1)!} \left\{ \frac{3r\delta}{2 - r(2r+1)} \right\}. \tag{28}$$

The coefficients b_r take the form

$$b_r = \begin{cases} -2\Sigma_{s=0}^{(r-2)/2} \Delta_{r,s} & \text{for even } r \\ 2\Sigma_{s=0}^{(r-1)/2} \Delta_{r,s} - \dfrac{1}{(r^{\zeta})^2} \left\{ 1 - \dfrac{(r-1)(2r+3)\delta}{1 + r(r-1)\delta} \right\} & \text{for odd } r \end{cases}$$

where $\Delta_{r,s}$ is given by

$$\Delta_{r,s} = \frac{1}{(2s+1)!(2r-2s-1)!} \left\{ 1 + \frac{(r-1)(2r+3)\delta}{1 + r(r-1)\delta} \right\}.$$

6. Numerical results and discussion

Here we have deformed the SE by giving a nonstandard realization of the kinetic energy operator, which coincides with the corresponding operator in the standard SE when

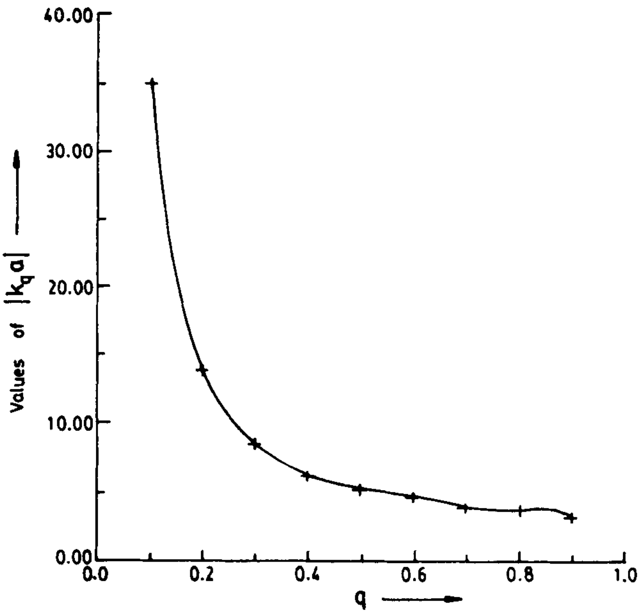

Figure 1. Variation of $|k_q a|$ (corresponding to the ground state) with q.

Table 1. Allowed values of $\pm k_q a$.

$q\downarrow n\rightarrow$	1	2	3	4
0·1	35·11869			
0·2	13·91709	69·87712		
0·3	8·564421	28·97956		
0·4	6·335347	16·46896	41·17533	
0·5	5·319289	10·92827	22·82981	45·21165
0·6	4·822798	8·039686	15·5551	24·57137
0·7	4·044871	7·795353	11·70577	15·03165
0·8	3·770396	7·872589	13·08165	14·74317
0·9	3·394796	6·803214	8·21286	

$q \rightarrow 1$. Numerical solutions of the q-SE for a particle in a box are obtained for values ranging from 0 to 1. It is observed that for lower values of q, higher energy levels are forbidden. This is due to the rapidly converging nature of the wavefunction for lower values of q. The numerical solutions are tabulated and the solution corresponding to the ground state of the system is plotted against q which is best fitted for a polynomial in q. The numerical solutions show that for $q \neq 1$, the energy eigenvalues have an upper bound even in systems which possess an infinite number of energy eigenvalues when $q = 1$.

Appendix 1

As the problem discussed in the text is a one dimensional one, all q-integrations are over a segment of finite length. The q-adjoint operation is defined as

$$S\phi_q^*(x)\Omega\psi_q(x)d(qx) = S(\Omega\phi_q(x))^*\psi_q(x)d(qx) \tag{A1}$$

where the functions $\phi_q(x)$ and $\psi_q(x)$ are assumed to vanish at the end points of the segment.

So a q-Hermitian operator Ω satisfies

$$S\phi_q^*(x)\Omega\psi_q(x)d(qx) = S(\Omega\phi_q(x))^*\psi_q(x)d(qx). \tag{A2}$$

A q-Hermitian operator has the following properties:

(i) The eigenvalues of a q-Hermitian operator are real.
Let $\Omega\psi_q(x) = \omega\psi(x)$ from (A2),

$$(\omega - \omega^*)S\psi_q^*(x)\psi_q(x)d(qx) = 0$$

which implies $\omega^* = \omega$.
(ii) The eigenvectors of a q-Hermitian operator belonging to different eigenvalues are q-orthogonal.

Suppose that $\psi_{q1}(x)$ and $\psi_{q2}(x)$ are two eigenvectors of Ω with eigenvalues ω_1 and ω_2 respectively.

$$S\psi_{q1}^*(x)\Omega\psi_{q2}(x)d(qx) = S(\Omega\psi_{q1}(x))^*\psi_{q2}(x)d(qx)$$

or,

$$(\omega_1 - \omega_2) S \psi_{q1}(x) \psi_{q2}(x) d(qx) = 0 \ (q\text{-orthogonality}).$$

Here we wish to show that $\mathbf{D}_x^2 \mathbf{q}^{-x\partial_x}$ is q-Hermitian:

$$\begin{aligned} S\phi_q^*(x)\mathbf{D}_x^2\mathbf{q}^{-x\partial_x}\psi_q(x)d(qx) &= S\phi_q^*(x)\mathbf{D}_x(\mathbf{D}_x\psi_q(q^{-1}x))d(qx) \\ &= |\phi_q^*(x)\mathbf{D}_x\psi_q(q^{-1}x)| - S\mathbf{D}_x\phi_q^*(x)q^{1/2}\mathbf{D}_x\psi_q(x)d(qx) \\ &= -q^{1/2}S\mathbf{D}_x\phi_q^*(x)\mathbf{D}_x\psi_q(x)d(qx) \end{aligned}$$

where we have employed the product rule for q-integration given by (7). Similarly,

$$S(\mathbf{D}_x^2\mathbf{q}^{-x\partial_x}\phi_q(x))^*\psi_q(x)d(qx) = -q^{1/2}S\mathbf{D}_x\phi_q^*(x)\mathbf{D}_x\psi_q(x)d(qx)$$

Thus $\mathbf{D}_x^2 \mathbf{q}^{-x\partial_x}$ is a q-Hermitian operator.

Acknowledgements

One of the authors (GV) thanks University Grants Commission for awarding a Research Fellowship. KMV would like to thank National Board of Higher Mathematics for awarding a post-doctoral fellowship.

References

[1] A Jannussis, L C Papaloucas and P D Sifarkas, *Hadronic J.* **3**, 1622 (1980)
[2] A Jannussis, G Brodinas and D Sourlas, *Lett. Nuovo Cimento* **30**, 123 (1981)
[3] L C Biedenharn, *J. Phys.* **A22**, L875 (1980)
[4] A J Macfarlane, *J. Phys.* **A22**, 4581 (1989)
[5] S Chaturvedi, A K Kapoor, R Sandhya, V Srinivasan and R Simon, *Phys. Rev.* **A43**, 4555 (1991)
[6] J A Minahan, *Mod. Phys. Lett.* **A5**, 2625 (1990)
[7] Yang Qin-Gzhu and Xu Bo-Wei, *J. Phys.* **A26**, L365 (1993)
[8] H Exton, *q-Hypergeometric functions and applications* (Chichester Ellis-Horwood, 1983)