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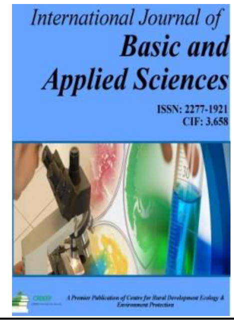

Full Length Research Paper

Orbital Angular Momentum in Oblate Spheroidal Coordinate

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ABSTRACT

The orbital angular momentum operators in quantum mechanics are best known in Cartesian and spherical coordinate. However, It is now well known that most common shapes of molecules, nucleus as well as the atom are not perfectly spherical as a result of deformation caused by competition between electromagnetic repulsion between protons, surface tension and quantum shell effects. Consequently, in this paper, we develop the orbital angular momentum operators and their commutation relation in the oblate spheroidal coordinate to pave way for the corresponding extension of the well-known orbital angular momentum in mechanics.

Introduction

It is well known how to formulate the angular momentum operators in spherical polar coordinate from the Cartesian coordinate in quantum mechanics. These operators are given by[1,2,3]

$$\hat{L}_x = i\hbar\left(\sin\phi\frac{\partial}{\partial\theta} + \cot\theta\cos\phi\frac{\partial}{\partial}\right) \qquad (1.1)$$

$$\hat{L}_y = i\hbar\left(-\cos\phi\frac{\partial}{\partial\theta} + \cot\theta\sin\phi\frac{\partial}{\partial}\right) \qquad (1.2)$$

$$\hat{L}_z = -i\hbar\frac{\partial}{\partial\phi} \qquad (1.3)$$

Then, the orbital angular momentum operator, $\hat{L}^2$ in the spherical polar coordinate is also given by[3];

$$\hat{L}^2 = -\hbar^2\left[\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right) + \frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\phi^2}\right] \qquad (1.4)$$

The corresponding eigenfunction for $\hat{L}^2$ operator is given by

$$-\hbar^2\left[\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right) + \frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\phi^2}\right]\psi = \lambda\psi \qquad (1.5)$$

On transformation, equation (1.5) gives an associate Legendre differential equation given by [3,5];

$$(1 - x^2)\Theta(x) - 2x\frac{d\Theta(x)}{dx} + \left(\frac{\lambda}{\hbar^2} - \frac{m^2}{(1-x^2)}\right)\Theta(x) = 0 \qquad (1.6)$$

Where λ is the eigenvalue given by [5];

$$\lambda = L(L+1)\hbar^2;\ L = 0,1,2,3,\ldots \qquad (1.7)$$

The corresponding normalized Eigenfunction is denoted by;

$$Y^m_{l(\theta,\phi)} = N_{lm}\, P^m_l(\cos\theta)\, e^{im\phi} \qquad (1.8)$$

Called the spherical harmonic function and N_{lm} is the normalization factor.

These equations constitute the basis of the study of the structures of atoms as well as other quantum problems that involve rotational symmetry. Also, the Eigenvalues and eigenfunction (spherical harmonics) of orbiting particles in quantum mechanicsare also determined using the angular momentum operators developed in the spherical coordinates [1,3,5,6]. It is most interesting to note that these equations were developed under the assumption that elementary particles such as electrons, molecules, atoms as well as nucleusexhibit perfect spherical symmetry due to their spherical shapes [3,6]. However, it is now well known experimentallythat the shape of most elementary particles as well as nuclei tends to be deformed due to quantum shell effects. The most commonly encountered shapes are elongated prolate or flattened oblate spheroidal [7]. Therefore, treating them as perfect spheres is at the best an approximation for the sake of mathematical conveniences. Therefore, there has remained the need to extend the theory of orbital angular momentum for orbiting particles of perfect spherical geometry to those of spheroidalgeometry. Consequently, in this paper we derived the orbital angular momentum operators and their commutation relations in the oblate spheroidal coordinate.

Mathematical formulations

The Cartesian coordinate (x, y, z) is related to the prolate spheroidal coordinate (η, ξ, ϕ) as [8,10];

$$x = a(1 - \eta^2)^{1/2}(1 + \xi^2)^{1/2}\cos\phi \qquad (1.9)$$

$$y = a(1 - \eta^2)^{1/2}(1 + \xi^2)^{1/2}\sin\phi \qquad (2.0)$$

$$z = a\eta\xi \qquad (2.1)$$

Where 'a' is the scale factor and

$$-1 \leq \eta \leq 1\,;\; 0 \leq \phi \leq 2\pi\,;\; 0 \leq \xi < \infty \qquad (2.2)$$

Similarly, the spherical polar coordinate (r, θ, ϕ) is related to the prolate spheroidal coordinate (η, ξ, ϕ) as;

$$r = a(1 + \eta^2 - \xi^2)^{1/2} \qquad (2.3)$$

$$\theta = \cos^{-1}\left(\frac{\eta\xi}{(1 + \eta^2 - \xi^2)^{1/2}}\right) \qquad (2.4)$$

$$\phi = \phi \qquad (2.5)$$

Therefore,

$$\frac{\partial r}{\partial x} = \frac{x}{r} \qquad (2.6)$$

$$\frac{\partial \eta}{\partial r} = \frac{(1 + \eta^2 - \xi^2)^{1/2}}{a\eta} \qquad (2.7)$$

$$\frac{\partial \xi}{\partial \theta} = \frac{-(1 - \eta^2)^{1/2}(1 + \eta^2 - \xi^2)}{\eta\,(1 + \eta^2)^{1/2}} \qquad (2.8)$$

$$\frac{\partial \theta}{\partial x} = \frac{x\eta\xi}{a^2(1 + \eta^2)^{1/2}\left(1 - \xi^2\right)^{1/2}(1 + \eta^2 - \xi^2)} \qquad (2.9)$$

$$\frac{\partial \phi}{\partial x} = \frac{-y}{a^2(1 + \eta^2)(1 - \xi^2)} \qquad (2.10)$$

$$\frac{\partial r}{\partial y} = \frac{y}{r} \qquad (2.10)$$

$$\frac{\partial \theta}{\partial y} = \frac{y\eta\xi}{a^2(1 + \eta^2)^{1/2}\left(1 - \xi^2\right)^{1/2}(1 + \eta^2 - \xi^2)} \qquad (2.11)$$

$$\frac{\partial \phi}{\partial y} = \frac{x}{a^2(1 + \eta^2)(1 - \xi^2)} \qquad (2.12)$$

$$\frac{\partial r}{\partial z} = \frac{z}{r} \qquad (2.13)$$

$$\frac{\partial \phi}{\partial z} = 0 \qquad (2.14)$$

$$\frac{\partial \theta}{\partial z} = \frac{-(1 + \eta^2)^{1/2}(1 - \xi^2)^{1/2}}{a(1 + \eta^2 - \xi^2)} \qquad (2.15)$$

It therefore follows from (2.8 – 3.8) that;

$$\frac{\partial}{\partial x} = \frac{x(1 + \eta^2 - \xi^2)^{1/2}}{a\eta\xi}\frac{\partial}{\partial \eta} - \frac{x\xi}{a^2(1 + \eta^2)^{1/2}}\frac{\partial}{\partial \xi} - \frac{y}{a^2(1 + \eta^2)(1 + \xi^2)}\frac{\partial}{\partial \phi} \qquad (2.16)$$

$$\frac{\partial}{\partial y} = \frac{y(1 + \eta^2 - \xi^2)^{1/2}}{a\eta\xi}\frac{\partial}{\partial \eta} - \frac{y\xi}{a^2(1 + \eta^2)^{1/2}}\frac{\partial}{\partial \xi} + \frac{x}{a^2(1 + \eta^2)(1 + \xi^2)}\frac{\partial}{\partial \phi} \qquad (2.17)$$

$$\frac{\partial}{\partial z} = \frac{z(1 + \eta^2 - \xi^2)^{1/2}}{a\eta\xi}\frac{\partial}{\partial \eta} - \frac{(1 - \xi^2)}{a\eta}\frac{\partial}{\partial \xi} \qquad (2.18)$$

The quantum orbital angular momentums are given in the Cartesian coordinate system as;

$$\hat{L}_x = -i\hbar\left(y\frac{\partial}{\partial z} - z\frac{\partial}{\partial y}\right) \qquad (2.19)$$

$$\hat{L}_y = -i\hbar\left(z\frac{\partial}{\partial x} - x\frac{\partial}{\partial z}\right) \qquad (2.20)$$

$$\hat{L}_z = -i\hbar\left(x\frac{\partial}{\partial y} - y\frac{\partial}{\partial x}\right) \qquad (2.21)$$

Equation (4.2 – 4.4) are transformed after series of mathematical manipulations as;

$$\hat{L}_{x(\eta,\xi,\phi)} = -i\hbar\left\{\frac{(1 - \xi^2)^{1/2}(\eta^2 + \xi^2 - 1)}{\eta(\eta^2 - 1)^{1/2}}\sin\phi\frac{\partial}{\partial \xi} - \frac{\eta\xi\cos\phi}{(1 - \eta^2)^{1/2}(\xi^2 - 1)^{1/2}}\frac{\partial}{\partial \phi}\right\} \qquad (2.22)$$

$$\hat{L}_{y(\eta,\xi,\phi)} = -i\hbar\left\{\frac{(1 - \xi^2)^{1/2}(\eta^2 + \xi^2 - 1)}{\eta(\eta^2 - 1)^{1/2}}\cos\phi\frac{\partial}{\partial \xi} - \frac{\eta\xi\sin\phi}{(1 - \eta^2)^{1/2}(\xi^2 - 1)^{1/2}}\frac{\partial}{\partial \phi}\right\} \qquad (2.23)$$

$$\hat{L}_{z(\eta,\xi,\phi)} = -i\hbar\frac{\partial}{\partial \phi} \qquad (2.24)$$

It therefore follows that the total angular momentum operator, $\hat{L}^2$ given by;

$$\hat{L}^2 = \hat{L}^2_x + \hat{L}^2_y + \hat{L}^2_z$$

Is obtained in the prolate spheroidal coordinate as;

$$\hat{L}^2 = -\hbar^2\left[\frac{(1-\xi^2)(1+\eta^2-\xi^2)^2}{\eta^2(1+\eta^2)}\frac{\partial^2}{\partial\xi^2} + \frac{(1+\eta^2-\xi^2)}{(1+\eta^2)(1-\xi^2)}\frac{\partial^2}{\partial\phi^2}\right] \quad (2.25)$$

Equation (4.5 – 4.7) represent the components of the orbital angular momentum operator in prolate spheroidal coordinate.

Commutation Relation

The quantum commutation relations were obtained using equation (2.25 – 2.28) as follows;

$$\left[\hat{L}_{x(\eta,\xi,\phi)}, \hat{L}_{y(\eta,\xi,\phi)}\right] = -i\hbar\left(\frac{\eta^2\xi^2}{(1+\eta^2)(1-\xi^2)}\right)\hat{L}_{z(\eta,\xi,\phi)} \quad (2.26)$$

$$\left[\hat{L}_{y(\eta,\xi,\phi)}, \hat{L}_{z(\eta,\xi,\phi)}\right] = i\hbar\hat{L}_{x(\eta,\xi,\phi)} \quad (2.27)$$

$$\left[\hat{L}_{z(\eta,\xi,\phi)}, \hat{L}_{x(\eta,\xi,\phi)}\right] = i\hbar\hat{L}_{y(\eta,\xi,\phi)} \quad (2.28)$$

$$\left[\hat{L}^2, \hat{L}_{x(\eta,\xi,\phi)}\right] = \left[\hat{L}^2, \hat{L}_{y(\eta,\xi,\phi)}\right] = \left[\hat{L}^2, \hat{L}_{z(\eta,\xi,\phi)}\right] = 0 \quad (2.29)$$

$$\left[\hat{L}_{x(\eta,\xi,\phi)}, x(\eta,\xi,\phi)\right] = -i\hbar\left[\frac{a\xi(1-\eta^2)^{1/2}(1-\xi^2)^{1/2}(\eta^2+\xi^2-1)\cos\phi\sin\phi}{\eta(\eta^2-1)^{1/2}(1+\xi^2)^{1/2}} + \frac{a\eta\xi(1+\xi^2)^{1/2}\cos\phi\sin\phi}{(1-\xi^2)^{1/2}}\right] \quad (2.30)$$

$$\left[\hat{L}_{y(\eta,\xi,\phi)}, y(\eta,\xi,\phi)\right] = -i\hbar\left[\frac{a\xi(1-\eta^2)^{1/2}(1-\xi^2)^{1/2}(\eta^2+\xi^2-1)\cos\phi\sin\phi}{\eta(\eta^2-1)^{1/2}(1+\xi^2)^{1/2}} + \frac{a\eta\xi(1+\xi^2)^{1/2}\cos^2\phi}{(1-\xi^2)^{1/2}}\right] \quad (2.31)$$

$$\left[\hat{L}_{z(\eta,\xi,\phi)}, z(\eta,\xi,\phi)\right] = 0 \quad (2.32)$$

Equations$(2.26-2.32)$ are the quantum commutation properties in the oblate spheroidal coordinate system(η,ξ,ϕ), which can now be compared to those of Cartesian and spherical polar coordinates to broaden insight into the uncertainty properties in orbital angular momentum.

Summary and conclusion

In this paper, we derived the components of the orbital angular momentum operator in the oblate spheroidal coordinate. We also derived the total angular momentum operator as well as the quantum commutation relations.

It is most interesting and instructive to note that the orbital angular momentum operators derived in this paper contain pure spheroidal terms and hence, has paved way for mathematical analysis and investigation into the structures of atoms, as well as other quantum problems that involve rotational symmetry.

It may be noted that equations (3.1 – 3.4), 3.7 obey the quantum commutation properties in the Cartesian and spherical polar coordinates. However, equation (3.5& 3.6) did not commute hence, $\hat{L}_{x(\eta,\xi,\phi)}, x(\eta,\xi,\phi)and\hat{L}_{y(\eta,\xi,\phi)}, y(\eta,\xi,\phi)$ are said to be complementary variables in the oblate spheroidal coordinate which cannot be measured simultaneously.

Finally, this has pave way for further research for the solution of the eigenfunction of$\hat{L}^2$, to explicitly determine the eigenvalues and eigenfunctions (spheroidal harmonics) of the oblate angular momentum where the spheroidal harmonics are the energy eigenfunctions of a particle whose configuration space is an oblate spheroidal.

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