Some intricacies of the momentum operator in quantum mechanics

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In quantum mechanics textbooks, the momentum operator is defined in Cartesian coordinates and the form of the momentum operator in spherical polar coordinates is rarely discussed. Consequently one always generalizes the Cartesian prescription to other coordinates and falls into a trap. In this work, we introduce the difficulties one faces when the question of the momentum operator in general curvilinear coordinates arises. We have tried to elucidate the points related to the definition of the momentum operator, taking spherical polar coordinates as our specimen coordinate system and proposing an elementary method in which we can ascertain the form of the momentum operator in general coordinate systems.

Keywords: Momentum operator; quantum mechanics.

En los libros de mecánica cuántica, el operador de momento se define en coordenadas cartesianas y raramente se discute la forma de este operador en coordenadas polares. En consecuencia, siempre se generaliza la prescripción de este operador en coordenadas cartesianas al caso de otras coordenadas con lo cual se suele caer en una trampa. En este trabajo, introducimos las dificultades que se encuentran cuando surge la pregunta de cómo se escribe el operador de momento en coordenadas curvilíneas generales. Tratamos de dilucidar los puntos relacionados con la definición del operador de momento tomado como ejemplo el caso de las coordenadas esféricas y proponemos un método elemental con el cual podemos establecer la forma del operador de momento en sistemas coordenados generales.

Descriptores: Operador de momento; mecánica cuántica.

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1. Introduction

In classical mechanics, the definition of momentum (both linear and angular) in Cartesian coordinates is simple. Linear momentum is defined as mass times velocity, and angular momentum is the cross-product of the position vector with the linear momentum vector of a particle or a body in motion. In classical mechanics, a particle must have a unique position and velocity and consequently the definition of momentum is unambiguous. When we are using generalized coordinates, then the definition of the generalized momenta straightforward. We have to know the Lagrangian $\mathcal{L}$ of the system written in the generalized coordinates, and the momentum conjugate to the generalized coordinate q_i is simply

$$p_i \equiv \frac{\partial \mathcal{L}}{\partial \dot{q}_i} \,. \tag{1}$$

In quantum mechanics the position of a particle is not unique; one has to revert to wave functions and then find out the probability density of finding the particle in some portion of space. Naturally the definition of momentum becomes a bit arbitrary. Elementary textbooks on quantum mechanics [1–3] invariably define the momentum operators in Cartesian coordinates, where ambiguities are fortunately fewer. In Cartesian coordinates we have three coordinates which have the same dimensions, and the linear momentum operator is defined as:

$$p_i = -i\hbar \frac{\partial}{\partial x_i} \,, \tag{2}$$

where $i = 1, 2, 3$. The angular momentum vectors are defined as:

$$L = -i\hbar(\mathbf{r} \times \nabla) \,. \tag{3}$$

All of the above definitions of momentum operators seem to be flawless in Cartesian coordinates. But one soon realizes that the definitions above are not all satisfatory if we have to generalize our results to various coordinate systems. In this article we shall illustrate the problems of defining the momentum operators in general curvilinear coordinates.

If we choose spherical polar coordinates, then the difficulty we face is that not all momentum components are of the same status (as in Cartesian coordinates), as one is a linear momentum and the other two are angular momenta. Moreover in quantum mechanics we do not have a relation corresponding to Eq. (1) to find out the momenta in arbitrary circumstances. The nice world of separate linear and angular momenta vanished and we must find how to define the momenta under these new circumstances. In addition to these difficulties we also have to consider whether the momentum operators defined are actually self-adjoint. In this article we shall not speak about the self-adjointness of the operators; for a better review on this topic, readers may consult [4]. In quantum mechanics, whenever we speak about angular momenta, in the back of our mind we conceive of the generators of rotation which follow the Lie algebra. But strictly speaking this fact is not true. In spherical polar coordinates,

$[p_\theta\,,\,p_\phi]=0$ although both of them are angular momentum operators. The Lie algebra of the angular momenta follows only when we are working in Cartesian coordinates.

In the present article, we try to formulate the important properties of the momentum operator which can be generalized to non-Cartesian coordinates, and in this process we point out which properties cannot be generalized. We try to treat both angular and linear momenta on the same footing and try to find out the properties of these operators. In the following section, we start with a general discussion of the momentum operator. Section 3 is dedicated to a description of the momentum operator in the Cartesian and the spherical polar coordinate systems, but its content is general and can be used to understand the form of the momentum operators in other coordinates as well. We conclude with a brief discussion on the topics described in the article in Sec. 4.

2. The momentum operator

Particularly in this section when we speak of momentum we shall not distinguish between linear and angular momenta. The coordinate system in which the position and momentum operators are represented is general with no bias in favour of the Cartesian system. The basic commutation relations in quantum mechanics are:

$$[q_i\,,\,p_j]=i\hbar\delta_{ij}\,, \tag{4}$$

and

$$[q_i\,,\,q_j]=[p_i\,,\,p_j]=0 \tag{5}$$

where q_j and p_j are the generalized coordinate and momentum operator and $\delta_{i\,j}=1$ when $i=j$ and zero for all other cases, and $i,j=1,2,3$. From Eq. (4) we can infer that the most general form of the momentum operator in quantum mechanics, in position representation, is:

$$p_i=-i\hbar\left[\frac{1}{f(q)}\frac{\partial}{\partial q_i}f(q)+h_i(q)+c_i\right]\,, \tag{6}$$

where $f(q)$ and $h_i(q)$ are arbitrary functions of coordinates q, and c_i are constants all of which may be different for different components of the momenta p_i. If we put this general form of the momentum operator into Eq. (5) we see that it restricts $h(q)$ to being a constant and so the general form of the momentum operator must be:

$$p_i=-i\hbar\left[\frac{1}{f(q)}\frac{\partial}{\partial q_i}f(q)+c_i\right]\,. \tag{7}$$

The form of $f(q)$ is arbitrary and has to be determined in different circumstances. In this article we show that one of the ways in which the function $f(q)$ can be determined is by imposing the condition that the momentum operator must have a real expectation value. The expectation value of the momentum operator is given as:

$$\langle p_i\rangle\equiv\int\sqrt{-g(q)}\,\psi^*(q)\,p_i\,\psi(q)\;d^3q\,, \tag{8}$$

where $g(q)$ is the determinant of the metric of the three-dimensional space. The constant c_i in the general form of the momentum operator in Eq. (7) turns out to be zero. Before going into the actual proof of the last statement, it should be noted that in any arbitrary coordinate system some of the canonical conjugate momenta will be linear and some will be angular. As the expectation values of the canonical momentum operators must be real, so for bound quantum states the expectation value of the linear momentum operators must be zero in any arbitrary coordinate system. Physically this means that coordinates with linear dimensions are in general non-compact and extend to infinity and for bound states, if the expectation value of the momenta conjugate to those non-compact coordinates is not zero, then it implies a momentum flow to infinity, which contradicts the very essence of a bound state. On the other hand, in an arbitrary coordinate system the expectation values of the angular momentum operators for any bound/free quantum state can be zero or of the form $M\hbar$ (from purely dimensional grounds), where M can be any integer (positive or negative) including zero. To prove that $c_i=0$, we first take those components of the momentum operator for which its expectation value turns out to be zero in an arbitrary coordinate system for a bound quantum state. Choosing those specific components of the momentum, we assume that for these cases $c_i\neq 0$ and it has a unique value. The value of c_i may depend on our coordinate choice but in any one coordinate system it must be unique. Suppose in the special coordinate system q the normalized wave function of an arbitrary bound state is given by $\psi(q)$. Then, from the definition of the general momentum operator in Eq. (7) this implies:

$$\langle p_i\rangle=0=-i\hbar F[\psi(q)]+c_i\,, \tag{9}$$

where $F[\psi(q)]$ is a functional of $\psi(q)$ given by:

$$F[\psi(q)]=\int\sqrt{-g(q)}\psi^*(q)\left[\frac{1}{f(q)}\frac{\partial}{\partial q_i}\{f(q)\psi(q)\}\right]d^3q, \tag{10}$$

which depends on the functional form of $\psi(q)$. If we choose another bound state in the same coordinate system whose normalized wave function is given by $\phi(q)$ then we can also write

$$-i\hbar F[\phi(q)]+c_i=0\,. \tag{11}$$

Comparing Eq. (9) and Eq. (11) we see that the value of c_i does not remain unique. The only way out is that c_i must be zero at least for those components of the momentum operator that have vanishing expectation values in bound states. Next we take those components of the momentum operator whose expectation values are of the form $M\hbar$. In these case also we can take two arbitrary but different bound state wave-functions $\psi(q)$ and $\phi(q)$. Evaluating $\langle p_i\rangle$ using these two different wave-functions will yield two similar spectra of

momenta as $M\hbar$ and $N\hbar$ where M and N belong to the set of integers including zero. In this case also we see that two quantum systems with different wave-functions yield similar momentum expectation values. Consequently in this case also we must have $c_i = 0$, otherwise it will not be unique. Although we utilized some properties of bound systems in quantum mechanics to show that $c_i = 0$ in general, we assume that the form of the canonical momentum operator is the same for bound and free quantum states. Thus the most general form of the canonical momentum operator for any quantum mechanical system in any coordinate system must be of the form:

$$p_i = -i\hbar \frac{1}{f(q)} \frac{\partial}{\partial q_i} f(q), \tag{12}$$

which still contains the arbitrary function $f(q)$ whose form is coordinate system dependent. From Eq. (6) we dropped the function $h_i(q)$ because the momentum components must satisfy $[p_i\,,\,p_j] = 0$. The last condition is not always true as in the case of charged particles in the presence of an external classical electromagnetic field. For charged particles in the presence of a classical external electromagnetic field the momentum components do not commute and in those cases the most general form of the momentum operator will contain $h_i(q)$ as in Eq. (6) while c_i will be zero. In presence of an electromagnetic field the momenta components of the electron are defined in the Cartesian coordinates as

$$\pi_i \equiv -i\hbar \frac{\partial}{\partial x_i} + ieA_i(\mathbf{x}),$$

where e is the negative electronic charge and $A_i(\mathbf{x})$ is the electromagnetic gauge field. In this case $[\pi_i\,,\,\pi_j] = -ieF_{ij}$ where F_{ij} is the electromagnetic field-strength tensor. As seen in these cases $h_i(q)$ will be proportional to the electromagnetic gauge field.

In this article, we assume that the form of the momentum operator in general orthogonal curvilinear coordinate systems is dictated by the basic commutation relations as given in Eq. (4) and Eq. (5) and the condition that the expectation value of the momentum operator must be real in any coordinate system. To find out the form of $f(q)$ we shall follow a heuristic method. A more formal approach to something similar to the topics discussed in this article can be found in Refs. 5 and 6. As the present article is purely pedagogical in intent we shall try to follow the path as (probably) taken by young graduate students who generalize the concepts of the Cartesian coordinates to any other coordinate system and in doing so fall into a trap. Then after some thinking the student understands the error in his/her thought process and mends his/her way to proceed towards the correct result. Consequently, the ansatz which we shall follow to find out the form of $f(q)$ is the following. First we will blindly assume, in any specific coordinate system, that $f(q) = 1$ as in the Cartesian coordinates and try to see whether the momentum operator yields a real expectation value. If this choice of $f(q)$ produces a real expectation value of the momentum operator, then the choice is perfect and we have the desired form of the momentum operator. If on the other hand with our initial choice of $f(q) = 1$ we do not get a real expectation value of the momentum operator, then we shall choose an appropriate value for it so that the redefined momentum yields real expectation values. In the cases which we shall consider in this article the form of $f(q)$ will be evident as soon as we demand that the momentum operators must have real expectation values.

In this article we assume that in general the wave functions we deal with are normalized to unity and the coordinate systems to be orthogonal. Moreover the wave functions are assumed to vanish at the boundaries or satisfy periodic boundary conditions.

3. The momentum operator in various coordinate systems

3.1. Cartesian coordinates

According to our ansatz here we initially take $f(x, y, z) = 1$, which implies that the x component of the momentum operator is as given in Eq. (2). If the normalized wave function solution of the time-independent Schrödinger equation of any quantum system is given by $\psi(\mathbf{x})$, where $\psi(\mathbf{x})$ vanishes at the boundaries of the region of interest, the expectation value of p_x is:

$$\begin{aligned}\int \psi^*(\mathbf{x})\, p_x\, \psi(\mathbf{x})\, d^3x &= -i\hbar \int\int dy\, dz \left[\int_{-L}^{L} \psi^*(\mathbf{x}, t)\, \frac{\partial \psi(\mathbf{x})}{\partial x}\, dx \right] \\ &= -i\hbar \int\int dy\, dz \left[\psi^*(\mathbf{x})\psi(\mathbf{x})|_{-L}^{L} - \int_{-L}^{L} \psi(\mathbf{x}) \frac{\partial \psi^*(\mathbf{x})}{\partial x}\, dx \right]. \end{aligned} \tag{13}$$

If the wave function vanishes at the boundaries L and $-L$ or are periodic or anti-periodic at those points, then the first term on the second line on the right-hand side of the above equation drops and we have,

$$\int \psi^*(\mathbf{x})\, p_x\, \psi(\mathbf{x})\, d^3x = -i\hbar \int\int dy\, dz \left[\int_{-L}^{L} \psi^*(\mathbf{x})\, \frac{\partial \psi(\mathbf{x})}{\partial x}\, dx\right]$$
$$= i\hbar \int\int dy\, dz \left[\int_{-L}^{L} \psi(\mathbf{x}) \frac{\partial \psi^*(\mathbf{x})}{\partial x}\, dx\right] = \int \psi(\mathbf{x})\, p_x^*\, \psi^*(\mathbf{x})\, d^3x\,. \quad (14)$$

This shows that the expectation value of p_x is real and so in Cartesian coordinates we have $f(x,y,z) = 1$. In a similar way it can be shown that with the same choice of $f(x,y,z)$ the expectation values of p_y and p_z are also real. The above analysis can also be done when the wave functions are separable. Consequently in Cartesian coordinates the momentum operators are given as in Eq. (2).

3.2. Spherical polar coordinates

3.2.1. The radial momentum operator

If we start with $f(r,\theta,\phi) = 1$ then the radial momentum operator looks like:

$$p'_r = -i\hbar \frac{\partial}{\partial r}\,. \quad (15)$$

If the solution of the time-independent Schrödinger equation for any particular potential is $\psi(r,\theta,\phi) \equiv \psi(\mathbf{r})$, then the expectation value of p'_r is

$$\langle p'_r \rangle = -i\hbar \int d\Omega \left[\int_0^\infty r^2\, \psi^*(\mathbf{r})\, \frac{\partial\, \psi(\mathbf{r})}{\partial r}\, dr\right], \quad (16)$$

where $d\Omega = \sin\theta\, d\theta\, d\phi$ and consequently,

$$\langle p'_r \rangle = -i\hbar \int d\Omega \left[\int_0^\infty r^2 \psi^*(\mathbf{r}) \frac{\partial \psi(\mathbf{r})}{\partial r}\, dr\right]$$
$$= -i\hbar \int d\Omega \left[r^2 \psi^*(\mathbf{r}) \psi(\mathbf{r})\big|_0^\infty - \int_0^\infty \left(2r\psi^*(\mathbf{r}) + r^2 \frac{\partial \psi^*(\mathbf{r})}{\partial r}\right) \psi(\mathbf{r})\, dr\right]. \quad (17)$$

If $\psi(\mathbf{r})$ vanishes as $r \to \infty$ then the above equation reduces to

$$\langle p'_r \rangle = i\hbar \int d\Omega \left[\int_0^\infty r^2 \psi(\mathbf{r}) \frac{\partial \psi^*(\mathbf{r})}{\partial r}\, dr\right] + 2i\hbar \int d\Omega \int_0^\infty r|\psi(\mathbf{r})|^2\, dr$$
$$= \langle p'_r \rangle^* + 2i\hbar \int d\Omega \int_0^\infty r|\psi(\mathbf{r})|^2\, dr\,. \quad (18)$$

The above equation implies that $\langle p'_r \rangle$ is not real in spherical polar coordinates. On the other hand if we write Eq. (18) as:

$$\langle p'_r \rangle - i\hbar \int d\Omega \int_0^\infty r|\psi(\mathbf{r}))|^2\, dr = \langle p'_r \rangle^* + i\hbar \int d\Omega \int_0^\infty r|\psi(\mathbf{r}))|^2\, dr\,, \quad (19)$$

then the left-hand side of the above equation can be written as:

$$\langle p'_r \rangle - i\hbar \int d\Omega \int_0^\infty r|\psi(\mathbf{r})|^2\, dr$$
$$= -i\hbar \int d\Omega \int_0^\infty \left[r^2 \psi^*(\mathbf{r}) \frac{\partial \psi(\mathbf{r})}{\partial r} + r|\psi(\mathbf{r})|^2\right] dr$$
$$= -i\hbar \int d\Omega \int_0^\infty r^2 \psi^*(\mathbf{r}) \left[\frac{\partial}{\partial r} + \frac{1}{r}\right] \psi(\mathbf{r})\, dr\,. \quad (20)$$

A similar manipulation on the right side of Eq. (19) can be done and it yields:

$$\langle p'_r \rangle^* + i\hbar \int d\Omega \int_0^\infty r|\psi(\mathbf{r})|^2\, dr$$
$$= i\hbar \int d\Omega \int_0^\infty \left[r^2 \psi(\mathbf{r}) \frac{\partial \psi^*(\mathbf{r})}{\partial r} + r|\psi(\mathbf{r})|^2\right] dr$$
$$= i\hbar \int d\Omega \int_0^\infty r^2 \psi(\mathbf{r}) \left[\frac{\partial}{\partial r} + \frac{1}{r}\right] \psi^*(\mathbf{r})\, dr\,. \quad (21)$$

Now if we redefine the radial momentum operator as:

$$p_r \equiv p'_r - \frac{i\hbar}{r} = -i\hbar \left(\frac{\partial}{\partial r} + \frac{1}{r}\right) = -i\hbar \frac{1}{r} \frac{\partial}{\partial r}\, r\,, \quad (22)$$

then from Eq.(19) we observe that the expectation value of p_r must have real values. This fact was derived in a different way by Dirac [7, 8]. Now this form of p_r we can identify as $f(r,\theta,\phi) = r$ in Eq. (7).

We end our discussion on the radial component of the momentum operator with an interesting example. Here we shall calculate the expectation value of the radial component of the force acting on an electron in the Hydrogen atom. The main purpose of this exercise is to generalize Heisenberg's equation of motion in spherical polar coordinates, which is not found in the elementary quantum mechanics text books. Although in the Heisenberg picture we deal with operators, to specify the relevant quantum numbers we first write down the wave-function of the Hydrogen atom explicitly. In the present case the wave-function is separable and it is given as:

$$\begin{aligned}\psi_{nLM}(r,\theta,\phi) &= N_r R_{nL}(r) Y_{LM}(\theta,\phi),\\ &= N_r e^{-r/na_0}\left[\frac{2r}{na_0}\right]^L \mathcal{L}^{2L+1}_{n-L-1}\\ &\times\left(\frac{2r}{na_0}\right) Y_{LM}(\theta,\phi), \end{aligned} \tag{23}$$

where $a_0 = \hbar^2/me^2$ is the Bohr radius and m is the reduced mass of the system comprising the proton and the electron, n is the principal quantum number which is a positive integer, $\mathcal{L}^{2L+1}_{n-L-1}(x)$ are the associated Laguerre polynomials, $Y_{L\,M}(\theta,\phi)$ are the spherical-harmonics, and N_r is the normalization arising from the radial part of the eigenfunction. The domain of L is made up of positive integers including zero and M are such that for each L, $-L \le M \le L$. The radial normalization constant is given by:

$$N_r = \left[\left(\frac{2}{na_0}\right)^3 \frac{(n-L-1)!}{(n+L)!2n}\right]^{1/2}. \tag{24}$$

The spherical-harmonics are given by,

$$\begin{aligned}Y_{L\,M}(\theta,\phi) &= (-1)^M \left[\frac{2\,L+1}{4\pi}\frac{(L-M)!}{(L+M)!}\right]^{1/2}\\ &\times P^L_M(\cos\theta) e^{iM\phi}\,, \end{aligned} \tag{25}$$

where $P^M_L(\cos\theta)$ are the associated Legendre functions.

From elementary quantum mechanics textbooks we know that in Cartesian coordinates the time evolution of the momentum operator in one dimension is given as:

$$\frac{dp_x}{dt} = \frac{1}{i\hbar}[p_x, H] = -\frac{d}{dx}V(x)\,, \tag{26}$$

which is the operator version of Newton's second law. Now if we take the expectation values of both sides of Eq. (26) in any basis we get:

$$\frac{d\langle p_x\rangle}{dt} = -\left\langle \frac{d}{dx}V(x)\right\rangle, \tag{27}$$

which is called the Ehrenfest theorem. In the case of the Hydrogen atom $V(\mathbf{r}) = -e^2/r$ and if we follow the Cartesian prescription we shall write,

$$\frac{dp_r}{dt} = -\frac{d}{dr}V(r) = -\frac{e^2}{r^2}\,, \tag{28}$$

which implies that the only force acting on the electron is the centripetal force supplied by the Coulomb field. But the above equation presents some difficulties. First from our knowledge of particle mechanics in central force fields we know that there must be some centrifugal reaction also which is absent in Eq. (28). Secondly as the Hydrogen atom is a bound system, the expectation value of its radial component of the momentum vanishes and consequently the time rate of change of the radial momentum expectation value must also vanish. But if we take the expectation value of the right-hand side of Eq. (28) it does not vanish. So Eq. (28) is a wrong equation and we cannot blindly use the Cartesian prescription in such a case.

The correct way to proceed in the present circumstance is to write Heisenberg's equation of motion in spherical polar coordinates using Eq. (22) as the radial momentum operator. In this way we will get all the results right. The Hamiltonian of the Hydrogen atom is:

$$H = -\frac{\hbar^2}{2m}\frac{1}{r}\frac{\partial^2}{\partial r^2}\,r + \frac{1}{2mr^2}\mathbf{L}^2 - \frac{e^2}{r}\,, \tag{29}$$

where,

$$\mathbf{L}^2 = -\hbar^2\left(\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\sin\theta\frac{\partial}{\partial\theta} + \frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\phi^2}\right), \tag{30}$$

whose eigenvalues are of the form $\hbar^2 L(L+1)$ in the basis $Y_{L\,M}(\theta,\phi)$. In the expression of the Hamiltonian m is the reduced mass of the system comprising the proton and electron. Next we try to apply Heisenberg's equation to the radial momentum operator. Noting that the first term of the Hamiltonian is nothing but p_r^2 the Heisenberg equation is:

$$\begin{aligned}\frac{dp_r}{dt} &= -\frac{\mathbf{L}^2}{2m}\left[\frac{1}{r}\frac{\partial}{\partial r}\,r\,,\,\frac{1}{r^2}\right] + e^2\left[\frac{1}{r}\frac{\partial}{\partial r}\,r\;,\,\frac{1}{r}\right],\\ &= \frac{\mathbf{L}^2}{mr^3} - \frac{e^2}{r^2}\,. \end{aligned} \tag{31}$$

The above equation is the operator form of Newton's second law in spherical polar coordinates. The first term on the right-hand side of the above equation gives the centrifugal reaction term in a central force field. Evaluating the expectation value of both the sides of the above equation using the wave-functions given in Eq. (23) we get [1],

$$\left\langle\frac{1}{r^2}\right\rangle = \frac{1}{n^3\,a_0^2(L+\frac{1}{2})}\,, \tag{32}$$

$$\left\langle\frac{1}{r^3}\right\rangle = \frac{1}{a_0^3\,n^3 L(L+\frac{1}{2})(L+1)}\,. \tag{33}$$

Using the above expectation values in Eq. (31) and noting that $\langle\mathbf{L}^2\rangle = \hbar^2 L(L+1)$ we see that the time derivative of the expectation value of the radial momentum operator of the Hydrogen atom vanishes. The interesting property to note is that, although the Heisenberg equation of motion for p_r shows that a force is acting on the system due to which p_r is changing, as soon we go to the level of expectation values the

force equation collapses to give a trivial identity. The cause of this is the reality of the radial momentum operator, which is bound to have a real value.

3.2.2. *The angular momentum operator canonically conjugate to ϕ and θ*

The canonically conjugate momenta corresponding to the angular variables must be angular momentum operators. Let p_ϕ be the angular momentum operator canonically conjugate to ϕ. In this case if we set $f(r,\theta,\phi) = 1$ the form of the momentum operator is:

$$p_\phi = -i\hbar\frac{\partial}{\partial\phi}\,, \tag{34}$$

which can be shown to posses real expectation values by following a similar proof to that of Eq. (13) and Eq. (14), if we assume $\Phi(0) = \Phi(2\pi)$. The periodic boundary condition forces the solution to the time-independent Schrödinger equation to be of the form:

$$\psi(r,\theta,\phi) \propto \frac{1}{\sqrt{2\pi}}\, e^{iM\phi}\,, \tag{35}$$

where $M = 0, \pm1, \pm2, \cdots$. The solution cannot have any other form of M dependence as in that case the expectation value of L_ϕ will not be of the form $M\hbar$. So for the case of ϕ, our initial choice of $f(r,\theta,\phi) = 1$ turns out to be correct.

Next we compute the expectation value of p_θ with $f(r,\theta,\phi) = 1$. The expectation value of $\langle p_\theta\rangle$ is as follows:

$$\begin{aligned}
\langle p_\theta\rangle &= -i\hbar\int\int r^2 dr d\phi\left[\int_0^\pi \psi^*(\mathbf{r})\frac{\partial\psi(\mathbf{r})}{\partial\theta}\,\sin\theta d\theta\right]\\
&= -i\hbar\int\int r^2 dr d\phi\left[\sin\theta\,\psi^*(\mathbf{r})\psi(\mathbf{r})|_0^\pi - \int_0^\pi\left(\cos\theta\,\psi^*(\mathbf{r}) + \sin\theta\frac{\partial\psi^*(\mathbf{r})}{\partial\theta}\right)\psi(\mathbf{r})\,d\theta\right]\\
&= \int\int r^2 dr d\phi\left[i\hbar\int_0^\pi \sin\theta\,\psi(\mathbf{r})\frac{\partial\psi^*(\mathbf{r})}{\partial\theta}\,d\theta\right] + i\hbar\int\int r^2 dr d\phi\int_0^\pi\cos\theta\,|\psi(\mathbf{r})|^2\,d\theta\\
&= \langle L_\theta\rangle^* + i\hbar\int\int r^2 dr d\phi\int_0^\pi\cos\theta\,|\psi(\mathbf{r})|^2\,d\theta\,.
\end{aligned} \tag{36}$$

The above equation shows that $\langle p_\theta\rangle$ is not real and so our choice of $f(r,\theta,\phi)$ is not correct. Following similar steps as done for the radial momentum operator we can redefine the angular momentum operator conjugate to θ as [9]:

$$p_\theta \equiv -i\hbar\left(\frac{\partial}{\partial\theta} + \frac{1}{2}\cot\theta\right)\,. \tag{37}$$

From the form of p_θ we find that in this case $f(r,\theta,\phi) = \sqrt{\sin\theta}$ in Eq. (7).

3.2.3. *The signature of the unequal domain of the angular variables in spherical polar coordinates*

It is known that both θ and ϕ are compact variables, *i.e.*, they have a finite extent. But there is a difference between them. In spherical polar coordinates the ranges of ϕ and θ are not the same: $0 \le \phi < 2\pi$ and $0 \le \theta \le \pi$. This difference has an interesting result. Since ϕ runs over the whole angular range, the wave-function has to be periodic in nature, whereas due to the range of θ, the wave-function need not be periodic. Consequently there can be a net angular momentum along the ϕ direction while there cannot be any net angular momentum along the θ direction. Whatever the quantum system may be, we will always have the expectation value of p_θ equal to zero although the wave-functions may not be periodic in θ or it may not vanish at $\theta = 0$ and $\theta = \pi$. In this article we shall show the validity of this observation for those cases where the wave-functions are separable, but the result holds for non-separable wave-functions also.

The time-independent Schrödinger equation for a central potential yields the wave-function corresponding to θ as $\Theta(\theta)$, given by:

$$\Theta(\theta) = N_\theta\, P_M^L(\cos\theta)\,, \tag{38}$$

where N_θ is a normalization constant depending on L, M and $P_M^L(\cos\theta)$ is the associated Legendre function, which is real. In the above equation L and M are integers where $L = 0, 1, 2, 3, \cdot\cdot$ and $M = 0, \pm1, \pm2, \pm3, \cdot\cdot$. A requirement of the solution of the Schrödinger equation for a central potential is that $-L \le M \le L$. Now we can calculate the expectation value of p_θ using the above wave-function and it is:

$$\langle p_\theta \rangle = -i\hbar N_\theta^2 \int_0^\pi P_M^L(\cos\theta)\left(\frac{dP_M^L(\cos\theta)}{d\theta} + \frac{1}{2}\cot\theta P_M^L(\cos\theta)\right)\sin\theta d\theta$$
$$= -i\hbar N_\theta^2 \left[\int_0^\pi P_M^L(\cos\theta)\frac{dP_M^L(\cos\theta)}{d\theta}\sin\theta d\theta + \frac{1}{2}\int_0^\pi P_M^L(\cos\theta)P_M^L(\cos\theta)\cos\theta\, d\theta\right] . \quad (39)$$

To evaluate the integrals on the right-hand side of the above equation we can take $x = \cos\theta$ and then the expectation value becomes:

$$\langle p_\theta \rangle = -i\hbar N_\theta^2 \left[\int_1^{-1} P_M^L(x)\frac{dP_L^M(x)}{dx}(1-x^2)^{\frac{1}{2}}\, dx - \frac{1}{2}\int_1^{-1} P_{M(x)}^L P_{M(x)}^L \frac{x}{\sqrt{1-x^2}}dx\right] . \quad (40)$$

The second term on the right-hand side of the above equation vanishes as the integrand is an odd function in the integration range. For the first integral we use the following recurrence relation [10]:

$$(x^2-1)\frac{dP_M^L(x)}{dx} = MxP_M^L(x) - (L+M)P_{M-1}^L(x)\,, \quad (41)$$

the last integral can be written as

$$\langle p_\theta \rangle = i\hbar N_\theta^2 \left[M\int_1^{-1} x(1-x^2)^{-\frac{1}{2}} P_M^L(x)P_M^L(x)\, dx - (L+M)\int_1^{-1}(1-x^2)^{-\frac{1}{2}} P_M^L(x)P_{M-1}^L(x)dx\right] . \quad (42)$$

Since

$$P_M^L(x) = (-1)^{L+M}P_M^L(-x)\,, \quad (43)$$

we can see immediately that both integrands on the right-hand side of Eq. (42) are odd and consequently $\langle p_\theta \rangle = 0$ as expected. A similar analysis gives $\langle p_\phi \rangle = M\hbar$. As the motion along ϕ is closed, there can be a net flow of angular momentum along that direction; but because the motion along θ is not so, a net momentum along the θ direction will not conserve probability, and consequently for probability conservation we must have an expectation value for the angular momentum along this direction equal to zero.

4. Conclusion

Before concluding, we would like to point out that the form of the momentum operators in the other widely used curvilinear coordinates as the cylindrical polar coordinates or the plane polar coordinates can be found in the same way as for spherical polar coordinates. The form of the momentum operator in most of the commonly used coordinates can be deduced from the ansatz which we presented in Sec. 2. Although the treatment presented in this article is not a general technique which can be applied in all circumstance as in that case one has to proof that this process of fixing the form of the momentum is unique and can be applied to all coordinate systems, no matter how pathological they may be.

The points discussed above are rarely dealt with in elementary quantum mechanics textbooks. Most often the linear momentum operator is defined in Cartesian coordinates and it is intuitively attached to the generator of translations. The difficulty in such an approach is that it becomes very difficult to generalize it to other curvilinear coordinates where the concept of translation is non-trivial. Moreover in arbitrary coordinate systems the concept of the uncertainty of the position and momentum operators becomes a difficult and non-trivial concept. As curvilinear coordinates contain compact dimensions it may happen that the uncertainties in those directions exceed the domain of the coordinate for a sharply defined conjugate momentum and so the conventional understanding of the uncertainty relation in general breaks down.

In the present work, we have emphasized the reality of the momentum expectation value and using the reality of the expectation value as a bench mark we found the form of the momentum. Linear and angular momenta were not dealt with differently. This process of deduction is interesting as in most cases the actual expectation value of the momentum is zero. It may seem that the deductions were incorrect as we manipulated zeros. In this regard it must be understood that the actual expectation values of the momenta in bound state turns out to be zero in many cases because the expectation values are required to be real. As in bound state problems we have real wave-functions so the expectation value of the momenta operators can be real only when it is zero. Consequently the reality of the expectation value is a concept which is more important than the fact that in many cases the expectation value turns out to be zero. In the present work the same prescriptions which yield the forms of the linear momenta also gives us the forms of the angular momenta. It was shown that regardless of the nature of the potential, the expectation value of the angular momentum conjugate to θ in spherical polar coordinates is zero. This is more a geometric fact than a physical effect.

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1. J.J. Sakurai, *Modern quantum mechanics*, International student edition (Addison-Wesley, 1999).
2. LI. Schiff, *Quantum mechanics*, third edition (McGraw-Hill International Editions).
3. R. Shankar, *Principles of quantum mechanics*, second edition (Plenum Press, New York 1994).
4. G. Bonneau, J. Faraut, and G. Valent, *Am. J. Phys.* **69** (2001) 322.
5. B. Podolsky, *Phys. Rev.* **32** 1928 812.
6. B.S. DeWitt, *Phys. Rev.* **85** (1952) 653.
7. P.A.M Dirac. *The principles of quantum mechanics*, Fourth edition (Oxford University Press, 1958).
8. S. Flügge, *Practical quantum mechanics I* (Springer-Verlag Berlin Heidelberg, 1971).
9. H. Essén, *Am. J. Phys.* **46** (1978) 983.
10. I.S. Gradshteyn and I.M. Ryzhik, *Table of integrals, series, and products*, sixth edition (Academic Press, Harcourt India) p. 955 **8.733** 1.