Angular Momentum and the Two-Dimensional Free Particle

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The one-dimensional free particle is among the first examples of quantum system that students meet in quantum mechanics and quantum chemistry introductory textbooks (*1-5*). This simple system is widely employed as a *model* system which allows the teacher to introduce very important topics such as the Heisenberg principle, the concept of constant of motion and the solution of the Schrödinger equation in terms of plane waves. The three-dimensional free particle is sometimes studied soon after (*4*) or in conjunction with the theory of scattering (*5*). However, the algebra becomes rather intricate and the ability to plot the wavefunction in a simple manner is lost. In any case the parallels between the properties of the quantum system and those of the classical one are not fully perceived.

In this paper we wish to show that the quantum free particle has many interesting properties usually not mentioned in introductory books (most notably the existence and the conservation of angular momentum) and that it can be used to introduce the students to important topics often encountered much later in the course such as the expansion of the wavefunction on a complete basis and the transformation between different bases. The best compromise between the opposite requests of algebraic simplicity and physical interest is the two-dimensional free particle system. Atomic units ($h = 1$) are used throughout the paper.

The classical system

Before considering the properties of the quantum free particle, it is useful to briefly refresh our memories on its classical counterpart. A free particle is, by definition, not subject to any force or constraint, that is, the force acting upon it is $\mathbf{F} \equiv (F_x, F_y) = 0$ everywhere. The classical equation of motion is $\mathbf{F} = m\,\mathbf{a}$, where m is the constant mass of the particle and $\mathbf{a}$ is its acceleration. We can rewrite this equation defining the linear momentum $\mathbf{p} = m\mathbf{v}$ and using $\mathbf{a} = \frac{d\mathbf{v}}{dt}$; we thus obtain $\frac{d\mathbf{p}}{dt} = 0$. This means that the linear momentum $\mathbf{p}$ is a constant of motion, i. e., a quantity that does not change during the motion of the particle. Are there other constants of motion that characterize the particle? The kinetic energy of the particle $E = |\mathbf{p}|^2/2m = p^2/2m$ is clearly a constant of motion. Note that the kinetic energy coincides with the total energy as the particle is not subject to any potential.

Both in classical and in quantum mechanics a quantity that is of primary value in discussing the properties of the motion is the angular momentum. In two dimensions the angular momentum of the particle with respect to the origin of the reference frame is a scalar defined as $L = xp_y - yp_x$. It is easily proved that the angular momentum is conserved during the motion of the particle by differentiating its definition with respect to time and using $d\mathbf{p}/dt = 0$. There is then another constant of motion, in addition to the linear momentum and the total energy: the angular momentum. Also note that the conservation of the angular momentum is not related to rotation in the present case.

From the definition of the angular momentum, it is very easy to show that a free particle moving through the origin has a null angular momentum, whereas a particle with non-zero angular momentum does not pass through the origin. The minimum distance b between the particle and the origin is called "impact parameter" and is equal to $|L|/|\mathbf{p}|$. For our later discussion, it is important to note that by fixing the linear momentum $\mathbf{p}$ the velocity and the energy of the particle are determined, but this is not sufficient to completely determine the graph of the trajectory. To do so we need to specify also the angular momentum. In other words, fixing the energy amounts to fixing the magnitude of $\mathbf{p}$ but not its direction, but L is left completely unspecified, i. e., the energy and the angular momentum are independent of each other.

The quantum system

The total energy is associated to the Hamiltonian operator $\hat{H}$, that is written for the free particle system as

$$\hat{H} = \frac{\hat{p}^2}{2m} = -\frac{1}{2m}\left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2}\right) \tag{1}$$

When $\hat{H}$ does not depend explicitly on time, as in the present case, the total energy E is a constant of motion. The solutions of the stationary Schrödinger equation $\hat{H}\Psi = E\Psi$, i. e., the eigenfunctions of the Hamiltonian operator are the so-called plane waves

$$\Psi_{k_x,k_y}(x, y) = \frac{1}{2\pi} e^{i\left(k_x x + k_y y\right)} = \frac{1}{2\pi} e^{i\mathbf{k}\cdot\mathbf{r}} \tag{2}$$

where $\mathbf{r} = (x, y)$, k_x and k_y are real numbers and the factor $1/2\pi$ is a normalization constant which we will drop in the following discussion to avoid unnecessary cluttering of the equations. The eigenvalues are $E = \left(k_x^2 + k_y^2\right)/2m = k^2/2m$. There is no restriction on the values that k_x and k_y can assume, therefore the energy of a free particle is *not* quantized.

Now we turn to the linear momentum, which is associated to the two quantum operators

$$\hat{p}_x = -i\frac{\partial}{\partial x} \quad \text{and} \quad \hat{p}_y = -i\frac{\partial}{\partial y} \tag{3}$$

which form the vector operator $\hat{\mathbf{p}} = \left(\hat{p}_x, \hat{p}_y\right)$. Both components of the linear momentum operator commute with the Hamiltonian $[\hat{H}, \hat{p}_x] = [\hat{H}, \hat{p}_y] = 0$ and then we find again that the linear momentum is a constant of motion. It is noteworthy that the components of the linear momentum commute with each other. This means that all three operators can share the same set of eigenfunctions. These are the plane waves, in fact $\hat{p}_x \Psi_{k_x,k_y} = k_x \Psi_{k_x,k_y}$ and $\hat{p}_y \Psi_{k_x,k_y} = k_y \Psi_{k_x,k_y}$. The components of the vector $\mathbf{k}$ are then the eigenvalues of the linear momentum and since they can assume any real value, also the linear momentum is *not* quantized.

A particle described by Ψ_{k_x,k_y} is characterized by the eigenvalues E, k_x, and k_y, that is, it has well-defined linear momentum and energy. Note however that, being $E = k^2/2m$, the state is completely defined by specifying only k_x and k_y and then it is sufficient to denote such a state as Ψ_{k_x,k_y} rather than Ψ_{E,k_x,k_y}. The Ψ_{k_x,k_y} can be divided in subsets containing eigenfunctions which differ only in the *direction* of **k**. The eigenfunctions within each subset are said to be degenerate, i. e., they have the same energy but differ in one or more of the eigenvalues needed to completely determine the state of the system. The probability density $\left|\Psi_{1,0}\right|^2$ is constant on the whole x,y-plane. Being the linear momentum exactly defined, the Heisenberg principle tells us that we know nothing about the particle position, so any plane wave gives a constant probability density.

The eigenfunctions of the angular momentum

We have previously seen that the classical free particle has a constant angular momentum, so we should not be surprised that the angular momentum operator $\hat{L} = x\hat{p}_y - y\hat{p}_x = -i\left(x\dfrac{\partial}{\partial y} - y\dfrac{\partial}{\partial x}\right)$ commutes with the Hamiltonian operator. As before we can choose the solutions of the Schrödinger equation to be also eigenfunction of the angular momentum operator with eigenvalue l. However, $\hat{L}$ does not commute with $\hat{p}_x$ and $\hat{p}_y$, as can be easily checked, so these eigenfunctions represent a particle with well-defined energy but undefined linear momentum (we only know its magnitude $k = \sqrt{2mE}$ but not its direction). We then label the solutions as $\Psi_{E,l}$. On the other hand, Ψ_{k_x,k_y} represents a state with well-defined linear momentum but undefined angular momentum since it is not eigenfunction of $\hat{L}$.

In order to find $\Psi_{E,l}$ we begin by expressing the angular momentum operator in polar coordinates $r = \sqrt{x^2 + y^2}$ and $\varphi = \arctan(y/x)$:

$$\hat{L} = -i\left(x\frac{\partial}{\partial y} - y\frac{\partial}{\partial x}\right) = -i\frac{\partial}{\partial \varphi} \tag{4}$$

The general solution of the angular momentum eigenvalue equation

$$\hat{L}\Phi(\varphi) \equiv -i\frac{\partial}{\partial\varphi}\Phi(\varphi) = l\,\Phi(\varphi) \tag{5}$$

is $\Phi(\varphi) = e^{il\varphi}$ (note the resemblance with eq 2). We now require that $\Phi(\varphi + 2\pi) = \Phi(\varphi)$ since any physical system composed of particles is left unchanged by a rotation through 2π. Since $\Phi(\varphi + 2\pi) = \Phi(\varphi)\,e^{i2\pi l}$ we must impose the condition that $e^{i2\pi l} = 1$, and this leads to the condition that l can only assume the discrete values 0, ±1, ±2, ... In other words, the angular momentum *is* quantized because of a boundary condition that is imposed on physical grounds to the solutions of the differential equation 5. A circular motion of the system is not necessarily involved in the quantization of the angular momentum as students may be driven to think when the quantization of $\hat{L}$ is introduced for the particle-on-a-ring system.

Expressing also the Hamiltonian operator in polar coordinates we can rewrite the Schrödinger equation in such a way that its solution has the form $\Psi(r,\varphi) = R(r)\,\Phi(\varphi)$ where the radial function $R(r)$ must satisfy

$$-\frac{1}{2m}\left(\frac{\partial^2}{\partial r^2} + \frac{1}{r}\frac{\partial}{\partial r} - \frac{l^2}{r^2}\right)R(r) = E\;R(r) \tag{6}$$

The solution of this equation can be found by consulting a mathematics handbook or by using a symbolic algebra package like Maple (*6*) or Mathematica (*7*). The radial function turns out to be a Bessel function of integer order $R(r) = J_l(\sqrt{2mE}\,r)$ where the energy E of the particle is not quantized. A state with definite energy and angular momentum is then described by the wavefunction

$$\Psi_{E,l}(r,\varphi) = e^{il\varphi}J_l(\sqrt{2mE}\,r) = e^{il\varphi}J_l(k\,r) \qquad l = 0, \pm 1, \pm 2, \ldots \tag{7}$$

where E and l are the eigenvalues of $\hat{H}$ and $\hat{L}$ and the last equality holds since $E = k^2/2m$. Of course, two wavefunctions with the same eigenvalue E but with different l are degenerate. Equation 7 shows that the energy of the particle is independent of the angular momentum, just like we found in the classical case, but in contrast with the case of the particle moving on a ring.

The probability density $\left|\Psi_{E,l}\right|^2 = \left[J_l\left(\sqrt{2mE}\, r\right)\right]^2$ is isotropic, i. e., it does not depend on φ. The main difference with respect to $\left|\Psi_{k_x,k_y}\right|^2$ is that now we do know something about the particle position since the squared modulus of $\Psi_{E,l}$ is not constant. There are points where the probability of finding the particle is large, points where it is small, and even points where the particle cannot be found. For instance, the quantum particle can be found at the origin only when $l = 0$ just like the classical particle passes through the origin only when $L = 0$. We can also draw an interesting parallel with the classical case by considering the radial probability $RPD_{E,l}(r)\, dr$, i. e., the probability of finding the particle at a distance from the origin comprised between r and $r+dr$:

$$RPD_{E,l}(r) = \int_0^{2\pi} \left|\Psi_{E,l}(r,\varphi)\right|^2 r\, d\varphi = 2\pi r\, J_l^2(k\, r) \qquad (8)$$

Near the origin the Bessel function $J_l(kr)$ can be approximated by $(kr/2)^l/l!$ and then the radial probability density behaves like r^{2l+1}. $RPD(r)$ is very small inside a circle of radius $b_l(k) = |l|/|\mathbf{k}|$ and this implies that a particle described by $\Psi_{E,l}$ is practically unaffected by what happens inside the circle. In classical mechanics the minimum distance from the origin attained by the particle is the impact parameter $b = |L|/|\mathbf{p}|$, which exactly parallels the expression for $b_l(k)$ making the substitution $L \rightarrow l$, $\mathbf{p} \rightarrow \mathbf{k}$.

Back and forth between representations

The eigenfunctions of the Hamiltonian operator always form a complete basis, so we can expand a generic state of the particle using either the plane waves of eq 2 or the functions with definite angular momentum of eq 7. This means that we can expand an eigenfunction with definite linear momentum using eigenfunctions with definite angular momentum, and vice versa. This is not a mere mathematical exercise but it has a physical meaning: suppose we prepare the particle in a state with definite energy and linear momentum, we can then ask what is the probability of finding a certain angular momentum as the outcome of an experiment.

Likewise we would like to know what is the probability of measuring a certain linear momentum for a particle having definite energy and angular momentum. To answer these questions we must look at the squared moduli of the expansion coefficients.
We begin by expanding a plane wave in eigenfunctions of the angular momentum:

$$\Psi_{k_x,k_y} = \sum_{l=-\infty}^{+\infty} i^l \, e^{-il\theta} \, \Psi_{E,l} \tag{9}$$

Note that the summation extends over all possible values of l, whereas the energy is restricted to the value $E = k^2/2m$, compatible with the magnitude k of the linear momentum. A state with a well-defined linear momentum **k** can be decomposed as a series of infinite states with fixed energy and well-defined angular momentum l. The squared modulus of any expansion coefficient is $\left| i^l e^{il\theta} \right|^2 = 1$, independent of l. This means that if we measure the angular momentum of a particle prepared as a plane wave we get as outcome any possible angular momentum with equal probability. This is analogous to the classical case where a particle with fixed energy and linear momentum can have any impact parameter and consequently any angular momentum.
Consider now a state with angular momentum l_0 and energy E. The formula that expands the eigenfunction of such a state over the functions Ψ_{k_x,k_y} is

$$\Psi_{E,l_0} = \frac{(-i)^{l_0}}{2\pi} \int_0^{2\pi} e^{il_0\theta} \, \Psi_{k_x,k_y} \, d\theta \tag{10}$$

Not all possible values of **k** are present under the integral: the integration is over all the *directions* that the vector **k** can assume while satisfying the condition $k^2 = E/2m$. This is analogous to the classical case, where for a given energy E there is an infinite number of **p** vectors which differ in orientation while satisfying $E = p^2/2m$. The squared modulus of any expansion coefficient is independent of **k** and therefore we reach a similar conclusion as before: measuring the linear momentum of a particle prepared with a definite energy and angular momentum can give as outcome any vector **k** with magnitude $k = \sqrt{2mE}$ with equal probability.

Conclusions

In this paper we have shown that the two-dimensional free particle is a system with many interesting properties that are not present in the one-dimensional case. This system, which can be treated at an elementary level, can be used to introduce the students to advanced concepts like the quantization of the angular momentum and the expansion of a wavefunction on a basis set.

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