Quantum mechanics in 3D and angular momentum

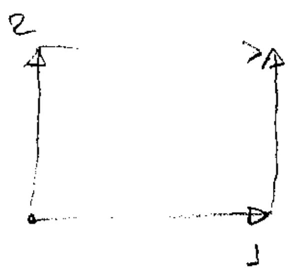
If we want to consider one particle in 3D, then we must consider 6 operators: $\hat{x}, \hat{y}, \hat{z}, \hat{p}_x, \hat{p}_y, \hat{p}_z$. It may be more convenient to name them $\hat{x}_1, \hat{x}_2, \hat{x}_3, \hat{p}_1, \hat{p}_2, \hat{p}_3$. The canonical commutation relations may now be written as

$$\boxed{[\hat{x}_j, \hat{p}_k] = i\hbar\, \delta_{jk}} \qquad (1)$$

and

$$[\hat{x}_j, \hat{x}_k] = [\hat{p}_j, \hat{p}_k] = 0 \qquad (2)$$

In words: a coordinate operator commutes with everything except its corresponding momenta. In a sense, (1) and (2) must be taken as a postulate. However, it is important to note that they make sense. For instance, if $[\hat{x}, \hat{y}] \neq 0$, then we would not be able to know the position of the particle that would be very strange. The same goes for $[\hat{p}_x, \hat{p}_y] \neq 0$. Recall that $\hat{p}$ is the generator of translation so that, if $[\hat{p}_x, \hat{p}_y] \neq 0$ the two paths below would not be equivalent



Eq (1) also holds when we have more than one particle. For N particles we have 3N operators $\hat{x}_1 \dots \hat{x}_{3N}$ and 3N momenta $\hat{p}_1 \dots \hat{p}_{3N}$. These operators obey the algebra of Eqs (1) and (2).

Wavefunction and Hamiltonians

The position ket for one particle in 3D is

$$|\vec{r}\rangle = |x, y, z\rangle = |x\rangle \otimes |y\rangle \otimes |z\rangle \tag{3}$$

If $|\alpha\rangle$ is some state of the particle, the corresponding wavefunction is

$$\psi(\vec{r}) = \langle \vec{r} | \alpha \rangle \tag{4}$$

It is normalized as

$$\int |\psi(\vec{r})|^2 d^3r = 1 \tag{5}$$

where

$$d^3r = dx\,dy\,dz \tag{6}$$

The dimension of ψ is therefore $1/L^{3/2}$.

Similarly, for N particles we have a position ket

$$|\vec{r}_1, \vec{r}_2, \ldots, \vec{r}_N\rangle \tag{7}$$

describing the position of N particles. The corresponding wavefunction is

$$\psi(\vec{r}_1, \ldots, \vec{r}_N) = \langle \vec{r}_1, \ldots \vec{r}_N | \alpha \rangle \tag{8}$$

It is normalized as

$$\int |\psi(\vec{r}_1 \ldots \vec{r}_N)|^2 d^3r_1 \ldots d^3r_N = 1 \tag{9}$$

This is a 3N-dimensional integral.

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The Hamiltonian for a single particle in 3D is the sum of kinetic and potential energy

$$\hat{H} = \frac{\vec{p}^{\,2}}{2m} + V(\vec{r}) \tag{10}$$

where $\vec{p} = (\hat{p}_x, \hat{p}_y, \hat{p}_z)$ so that (11)

$$\vec{p}^{\,2} = \hat{p}_x^2 + \hat{p}_y^2 + \hat{p}_z^2$$

If we wish to work in the ~~co~~ coordinate representation then we may write

$$\hat{p}_x = -i\hbar \frac{\partial}{\partial x} \tag{12}$$
$$\hat{p}_y = -i\hbar \frac{\partial}{\partial y}$$
$$\hat{p}_z = -i\hbar \frac{\partial}{\partial z}$$

A more compact way of writting this is to see that these derivatives are simply the components of the gradient

$$\boxed{\vec{p} = -i\hbar\nabla} \tag{13}$$

where

$$\nabla = \left(\frac{\partial}{\partial x}, \frac{\partial}{\partial y}, \frac{\partial}{\partial z}\right) \tag{14}$$

Accordingly, $\vec{p}^2$ will be the Laplacian

$$\vec{p}^{\,2} = -\hbar^2\nabla^2 = -\hbar^2\left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}\right) \tag{15}$$

Hence the Hamiltonian of a single particle in 3D is

$$\boxed{\hat{H} = -\frac{\hbar^2}{2m}\nabla^2 + V(\vec{r})} \tag{16}$$

The time-independent Schrödinger Eq is

$$\boxed{\hat{H}\,\psi(\vec{r}) = -\frac{\hbar^2}{2m}\nabla^2\psi(\vec{r}) + V(\vec{r})\psi(\vec{r}) = E\psi(\vec{r})} \tag{17}$$

nd the time dependent version is

$$i\hbar\frac{\partial\Psi(\vec{r},t)}{\partial t} = \hat{H}\Psi(\vec{r},t) \tag{18}$$

Example : free particle

The free particle in 1D has a Hamiltonian

$$\hat{H} = \frac{\hat{p}^2}{2m} \tag{19}$$

It is very easy to diagonalize this Hamiltonian because we know the eigenvalues and eigenvectors of $\hat{p}$:

$$\hat{p}\,|k\rangle = \hbar k\,|k\rangle \tag{20}$$

thus

$$\hat{H}\,|k\rangle = \frac{\hbar^2 k^2}{2m}\,|k\rangle \tag{21}$$

So the eigenvectors are $|k\rangle$ and the eigenvalues are $\frac{\hbar^2 k^2}{2m}$.

Now note something interesting: these energies are degenerate because k and $-k$ give the same energy. This degeneracy is a consequence of the fact that

$$[\hat{H}, \hat{p}] = 0 \tag{22}$$

This reflects a symmetry of the system. We will discuss this in more detail later. The corresponding wavefunction is

$$\phi_k(x) = \langle x|k\rangle = \frac{e^{ikx}}{\sqrt{2\pi}} \tag{23}$$

So the most general wavefunction with energy $\frac{\hbar^2 k^2}{2m}$ is

$$A\,e^{ikx} + B\,e^{-ikx} \tag{24}$$

Now consider a free particle in 3D. The Hamiltonian is

$$\hat{H} = \frac{\hat{p}_x^2}{2m} + \frac{\hat{p}_y^2}{2m} + \frac{\hat{p}_z^2}{2m} \tag{23}$$

Note that this Hamiltonian factors into 3 parts which commute. This is just like 3 non-interacting particles so that the eigenvectors will be

$$|\vec{k}\rangle = |k_x, k_y, k_z\rangle = |k_x\rangle \otimes |k_y\rangle \otimes |k_z\rangle \tag{24}$$

and the energies will be

$$E(\vec{k}) = \frac{\hbar^2 k^2}{2m} \tag{25}$$

where

$$k^2 = k_x^2 + k_y^2 + k_z^2 \tag{26}$$

The corresponding wavefunctions are

$$\phi_{\vec{k}}(\vec{r}) = \langle \vec{r} | \vec{k} \rangle = \left(\langle x| \otimes \langle y| \otimes \langle z|\right)\left(|k_x\rangle \otimes |k_y\rangle \otimes |k_z\rangle\right)$$

$$= \langle x | k_x\rangle \otimes \langle y | k_y\rangle \otimes \langle z | k_z\rangle$$

$$= \frac{e^{ik_x x}}{\sqrt{2\pi}} \frac{e^{ik_y y}}{\sqrt{2\pi}} \frac{e^{ik_z z}}{\sqrt{2\pi}}$$

or

$$\boxed{\phi_{\vec{k}}(\vec{r}) = \frac{e^{i\vec{k}\cdot\vec{r}}}{(2\pi)^{3/2}}} \qquad (2$$

which is a plane wave with momentum $\hbar\vec{k}$.

If we compare with the 1D problem, we now see that the degeneracy of each level is much larger. Essentially, to each value of energy $\frac{\hbar^2 k^2}{2m}$ there are an <u>infinite</u> <u>number</u> of vectors $\vec{k}$ (namely, all those vectors for which $|\vec{k}| = k$)

The reason behind this is that a free particle is <u>invariant under</u> <u>rotations</u>: the Hamiltonian has no preferred orientation so that if someone rotated your coordinate system, you wouldn't even know it.

This means that there must exist some unitary operator $\hat{D}$ which rotates the system and which commutes with the Hamiltonian. We will soon learn that this is related to angular momentum.

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It is also possible to solve the problem of the free particle using differential equations. This is not only much more laborious, but it is also blind about the symmetries of the problem. But in any case, I think once in your life you need to know how it is done. So I give this solution in Appendix A.

Example: 3D Harmonic oscillator.

The potential of a isotropic harmonic oscillator is

$$V(\vec{r}) = \frac{1}{2} m\omega^2 r^2 = \frac{1}{2} m\omega^2 (x^2 + y^2 + z^2) \qquad (28)$$

We will, however, consider the more general case of an anisotropic oscillator where

$$V(\vec{r}) = \frac{1}{2} m\omega_x^2 x^2 + \frac{1}{2} m\omega_y^2 y^2 + \frac{1}{2} m\omega_z^2 z^2 \qquad (29)$$

The total Hamiltonian is, therefore, a sum of 3 Hamiltonians

$$\hat{H} = \hat{H}_1 + \hat{H}_2 + \hat{H}_3 \qquad (30)$$

where

$$\hat{H}_j = \frac{\hat{P}_j^2}{2m} + \frac{1}{2} m\omega_j^2 \hat{x}_j^2 \qquad (31)$$

Notice that, due to (1) and (2), the 3 Hamiltonians commute with one another

$$[\hat{H}_1, \hat{H}_2] = [\hat{H}_1, \hat{H}_3] = [\hat{H}_2, \hat{H}_3] = 0 \qquad (32)$$

he system is thus identical to that of 3 non-interacting particles. We already know the eigenvalues and eigenvectors of each Hamiltonian since we know how o solve the problem of a single harmonic oscillator.

We have that

$$H_j \, | m_j \rangle = E^j_{m_j} \, | m_j \rangle \tag{33}$$

where $m_j = 0, 1, 2, \ldots$ and

$$E^j_{m_j} = \hbar \omega_j \left(m_j + 1/2 \right) \tag{34}$$

Since the total Hamiltonian is a sum, the eigenvectors of $\hat{H}$ will simply be the tensor product of the individual eigenvectors

$$| m_1, m_2, m_3 \rangle = | m_1 \rangle \otimes | m_2 \rangle \otimes | m_3 \rangle \tag{35}$$

the corresponding eigenvalues are

$$E(m_1, m_2, m_3) = \hbar \omega_1 (m_1 + 1/2) + \hbar \omega_2 (m_2 + 1/2) + \hbar \omega_3 (m_3 + 1/2) \quad (3$$

In the particular case of an isotropic oscillator we obtain

$$\boxed{E(m_1, m_2, m_3) = \hbar \omega \left(m_1 + m_2 + m_3 + 3/2 \right)} \quad (37$$

Note that there is a profound difference between the isotropic and the anisotropic oscillators, related to the degeneracy of each level. The table below analyzes the degeneracies of the isotropic energies in Eq (37):

Energy	Degeneracy	(n_x, n_y, n_z)
$\frac{3}{2}\hbar\omega$	$d_0 = 1$	$(0,0,0)$
$\frac{5}{2}\hbar\omega$	$d_1 = 3$	$(1,0,0)$, $(0,1,0)$, $(0,0,1)$
$\frac{7}{2}\hbar\omega$	$d_2 = 6$	$(2,0,0)$, $(0,2,0)$, $(0,0,2)$ $(1,1,0)$, $(1,0,1)$, $(0,1,1)$
$\frac{9}{2}\hbar\omega$	$d_3 = 10$	...

It can be shown that the degeneracy of the n-th level is

$$d_n = \frac{(n+1)(n+2)}{2} \tag{38}$$

Notice how these degeneracies do not appear in the anisotropic oscillator. They appear in the isotropic case due to a <u>symmetry</u> of this system. Namely, the isotropic oscillator is invariant under rotations, whereas the anisotropic oscillator is not. Symmetries usually lead to degeneracies.

Angular momentum

We have learned that the time-evolution operator is

$$\hat{U}(t) = e^{-i\hat{H}t/\hbar} \tag{39}$$

This operator takes a state $|\alpha(0)\rangle$ to a state $|\alpha(t)\rangle$

$$|\alpha(0)\rangle \xrightarrow{\hat{U}(t)} |\alpha(t)\rangle$$

We say $\hat{U}(t)$ performs a translation in time. The Hamiltonian is called the generator of time translations

Similarly you may recall the operator

$$\hat{T}(a) = e^{-i\hat{p}a/\hbar} \tag{40}$$

or its 3D version

$$\hat{T}(\vec{a}) = e^{-i\hat{\vec{p}}\cdot\vec{a}/\hbar} \tag{41}$$

We have shown that $\hat{T}$ performs translations in space. Accordingly, the operator $\hat{\vec{p}}$ is called the generator of spatial translations

I guess you see the pattern. Whenever we have a symmetry operation, we represent it by a unitary operator. This unitary operator is always the exponential of something times a Hermitian operator. We call this Hermitian operator the generator of the symmetry operation.

Complex systems have many symmetries and understanding them may greatly simplify the problem. The theory which systematically studies this is called group theory.

What we want to do now is study rotations. We will define a unitary operator $\hat{D}(\theta, n)$ such that

$$\hat{D}(\theta, n) = \text{rotates the system by an angle } \theta \text{ around the direction } n \tag{42}$$

You see: rotations are a bit trickier because you need an angle of rotation θ and a direction n around which you rotate (n is a unit vector).

We will soon learn that the generator of rotations is the angular momentum. It may not seem so now, but I guarantee you: understanding angular momentum will open your doors to a whole new world

The classical definition of angular momentum is

$$\vec{L} = \vec{r} \times \vec{p} \qquad (43)$$

There is nothing wrong with using this in quantum mechanics. But it is not the whole story. It turns out that in QM the definition of angular momentum is more general. For instance spin is a type of angular momentum but it cannot be written in the form of Eq (43).

We will thus use the following notation: when talking about ang. mom. in general we will use the letter $\vec{J}$. Terms like Eq (43) are called orbital angular momentum and will be denoted by the letter $\vec{L}$. Finally, spin angular momentum will be denoted by the letter $\vec{S}$.

In QM what really defines angular momentum are the commutation relations. Given any 3 operators $\hat{J}_x$, $\hat{J}_y$ and $\hat{J}_z$, we say that they correspond to angular momentum whenever they satisfy

$$\boxed{[\hat{J}_x, \hat{J}_y] = i\hbar \hat{J}_z \qquad [\hat{J}_y, \hat{J}_z] = i\hbar \hat{J}_x \qquad [\hat{J}_z, \hat{J}_x] = i\hbar \hat{J}_y} \qquad (44)$$

We will show in a second that this is indeed true for Eq (43). However, we leave this as a more general statement about angular momentum.

Before we analyze (43), let me make a few comments. Eq (44) are called the ang. mom. commutation relations or the ang. mom. algebra. Notice how they are cyclic in the 3 coordinates. If we write (1, 2, 3) instead of (x, y, z) we see that the formulas are always arranged as

$$1\ 2\ 3 \longrightarrow 3\ 1\ 2 \longrightarrow 2\ 3\ 1$$

It is also customary to write the 3 equations in (44) as

$$\boxed{[\hat{J}_i, \hat{J}_j] = i\hbar\, \epsilon_{ijk}\, \hat{J}_k} \tag{45}$$

where ϵ_{ijk} is the completely anti-symmetric Levi-Civita tensor defined as

$$\epsilon_{ijk} = \begin{cases} 0 & \text{repeated index} \\ 1 & \text{correct cyclic order: } 123,\ 312,\ 231 \\ -1 & \text{incorrect order} \end{cases} \tag{46}$$

Note also that a sum over k is implied in Eq (45). This is the Einstein summation rule commonly used in relativity: repeated indices are always summed.

There is one final comment to make: notice that ang. mom. has units of xp which is $\hbar$. Thus, it is convenient to, sometimes, define angular momentum in units of $\hbar$. For instance, Eq (43) could be defined as

$$\vec{L} := \frac{\vec{r} \times \vec{p}}{\hbar} \tag{47}$$

You will see that this greatly simplifies all equations. The commutation relations (45) become

$$\boxed{[\hat{J}_i, \hat{J}_j] = i\, \epsilon_{ijk}\, \hat{J}_k} \tag{48}$$

In this case angular momentum is dimensionless. We will actually change between the two conventions whenever is convenient. But don't worry, we will never be confused.

By the way, what we will show later is that the rotation operator (42) is actually

$$\boxed{\hat{D}(\theta, n) = e^{-i\theta\, n \cdot \vec{J}}} \tag{49}$$

so that the generator of rotations is, indeed, the angular momentum operator. Notice how it is very clear in Eq (49) that I am using $\vec{J}$ in units of $\hbar$. After all, the exponent must be dimensionless. Otherwise I would have to divide by $\hbar$.

Another comment: an even more compact way of writting Eq (48) is

$$\vec{J} \times \vec{J} = i \vec{J}$$

This used to be popular in older books, but for some reason people don't use it anymore. If $\vec{v}$ is a normal vector then $\vec{v} \times \vec{v} = 0$. But for vectors of operators this is not necessarily true.

$\vec{L}$ satisfies the angular momentum algebra

As promised, let us now verify that $\vec{L} = \vec{r} \times \vec{p}$ satisfies the angular momentum algebra in (45). In terms of components we have (I will drop hats for now)

$$L_x = y P_z - z P_y \tag{50a}$$

$$L_y = z P_x - x P_z \tag{50b}$$

$$L_z = x P_y - y P_x \tag{50c}$$

Note how there is no ambiguity about the order of each product. For instance, it doesn't matter if we write $y P_z$ or $P_z y$ because they commute.

Now I will check one of the commutation relations. The others then follow from the cyclic properties of the cross product. All we need is

$$[\hat{A}\hat{B}, \hat{C}] = \hat{A}[\hat{B}, \hat{C}] + [\hat{A}, \hat{C}]\hat{B} \tag{51}$$

We then have

$$[L_x, L_y] = [y P_z - z P_y, \; z P_x - x P_z]$$

$$= [y P_z, z P_x] - [y P_z, x P_z]$$

$$- [z P_y, z P_x] + [z P_y, x P_z]$$

In the two terms in the middle, everyone commutes with everyone. Thus

$$[y P_z, x P_z] = [z P_y, z P_x] = 0$$

As for the other terms, all that matters is $[z, P_z]$. Thus

$$[y P_z, z P_x] = y [P_z, z] P_x = -i\hbar\, y P_x$$

$$[z P_y, x P_z] = P_y [z, P_z] x = i\hbar\, x P_y$$

Thus we conclude that

$$[L_x, L_y] = i\hbar (x P_y - y P_x)$$

But looking back at (50c) we see that the right-hand side is simply L_z. Thus

$$[L_x, L_y] = i\hbar L_z$$

qed.

Appendix A: Alternative solution for the free particle

We wish to solve for the free particle in 3D using methods of differential equations. Thus, our goal is to solve

$$\frac{-\hbar^2}{2m}\left(\frac{\partial^2\psi}{\partial x^2}+\frac{\partial^2\psi}{\partial y^2}+\frac{\partial^2\psi}{\partial z^2}\right)=E\psi$$

or

$$\frac{\partial^2\psi}{\partial x^2}+\frac{\partial^2\psi}{\partial y^2}+\frac{\partial^2\psi}{\partial z^2}=-k^2\psi \tag{A.1}$$

where

$$k^2=\frac{2mE}{\hbar^2} \quad \text{or} \quad E=\frac{\hbar^2k^2}{2m} \tag{A.2}$$

Notice how I am assuming that E is positive. This must indeed be true since $\hat{H}=\frac{\hat{p}^2}{2m}$ and the eigenvalues of an operator squared must necessarily be non-negative.

Now I will use the favourite technique of anyone who solves partial differential equations: sepparation of variables. That is, I will use the Ansatz

$$\psi(x,y,z)=X(x)\,Y(y)\,Z(z) \tag{A.3}$$

ie, I will try to see if I can find solutions for which ψ is a product of functions, one of each argument

The neat thing about this ansatz is that, now, computing derivatives is simpler. For instance

$$\frac{\partial^2 \psi}{\partial x^2} = X''(x)\, Y(y)\, Z(z)$$

thus Eq (A.1) becomes

$$X'' Y Z + X Y'' Z + X Y Z'' = -k^2 X Y Z$$

Now comes the trick: since wavefunctions are never zero (unless we have infinite potentials, which we do not) then we may divide this equation by XYZ:

$$\boxed{\frac{X''(x)}{X(x)} + \frac{Y''(y)}{Y(y)} + \frac{Z''(z)}{Z(z)} = -k^2} \qquad (A.4$$

The left-hand side is a sum of 3 functions, one of x, one of y and one of z. But Eq (A.4) says that when you sum them the result is always a constant, $-k^2$. Thus, for any value of x, y and z that you choose, whenever you add up the particular combination in (A.4), you always get a constant. The only possibility is that each of the 3 functions must itself be a constant. Otherwise, this would never be true for arbitrary x, y, z. Hence

$$\frac{X''}{X} = -k_x^2 \qquad \frac{Y''}{Y} = -k_y^2 \qquad \frac{Z''}{Z} = -k_z^2$$

where k_x, k_y and k_z are constants such that

$$k_x^2 + k_y^2 + k_z^2 = k^2$$

(A.

Since the 3 Equations are identical we may simply solve for one of them, say x. We have

$$X''(x) = -k_x^2 X(x)$$

The solution of this Eq is

$$X(x) = A e^{i k_x x}$$

Thus, the general solution of the problem is

$$\psi(\vec{r}) = A e^{i \vec{k} \cdot \vec{r}}$$

where $\vec{k} = (k_x, k_y, k_z)$. The corresponding energies are

$$E(\vec{k}) = \frac{\hbar^2 k^2}{2m} = \frac{\hbar^2}{2m}(k_x^2 + k_y^2 + k_z^2)$$

A.4