33-234 Quantum Physics   Spring 2015

Derivation of Angular Momentum Rules in Quantum Mechanics
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These notes follow the derivation in the text but provide some additional details and alternate explanations. Comments are welcome.

For 33-234, you will not be responsible for the details of the derivations given here. We have covered the material necessary to follow the derivations so these details are presented for the ambitious and curious. All students should, however, be sure to understand the results as displayed on page 6 and following as well as the basic commutation properties given on this and the next page.

Classical angular momentum.   The classical angular momentum of a point particle is computed as

$$\mathbf{L} = \mathbf{R} \times \mathbf{p}, \tag{1}$$

where $\mathbf{R}$ is the position, $\mathbf{p}$ is the linear momentum. For circular motion, this reduces to $L = Rp = Rmv = \omega m R^2$ using $v = \frac{2\pi R}{T} = \omega R$. In the absence of external torques, $\mathbf{L}$ is a conserved quantity; in other words, it is constant in magnitude and direction. In the presence of a torque, τ (a vector quantity), generated by a force, $\mathbf{F}$, $\tau = \mathbf{R} \times \mathbf{F}$, the equation of motion is $\frac{d\mathbf{L}}{dt} = \tau$. In a composite system, the total angular momentum is computed as a vector sum: $\mathbf{L}_T = \sum_i \mathbf{L}_i$.

We would like to determine the stationary states of angular momentum and determine the "good" quantum numbers that describe these states. For a particle bound by some potential in three dimensions, we want to know the set of physical quantities that can be used to specify the stable states or eigenstates. We first make a quantum analog to (1) and then look for sets of operators that commute with each other so that they can have simultaneous eigenvalues.

Quantum operators and basic properties.   The basic translation to quantum mechanics is done by replacing the vector quantities in (1) with their operators; this then defines the angular momentum operator as follows:

$$\hat{\mathbf{L}} = \hat{\mathbf{R}} \times \hat{\mathbf{p}} \tag{2}$$

$$\hat{L}_x = \hat{y}\hat{p}_z - \hat{z}\hat{p}_y \tag{3}$$

$$\hat{L}_y = \hat{z}\hat{p}_x - \hat{x}\hat{p}_z \tag{4}$$

$$\hat{L}_z = \hat{x}\hat{p}_y - \hat{y}\hat{p}_x, \tag{5}$$

where equations 3 - 5 come from the evaluation of the cross product in (2). Note that the order in which the position-momentum products are written does not matter since $[r_\alpha, p_\beta] = i\hbar\delta_{\alpha\beta}$, with $\delta_{\alpha\beta}$ being the Kronecker delta function defined as $\delta_{\alpha\beta} = 0$ for $\alpha \neq \beta$ and $\delta_{\alpha\beta} = 1$ for $\alpha = \beta$.

Another operator of importance is the one yielding the magnitude of the angular momentum. We define

$$\hat{L}^2 = \hat{L}_x^2 + \hat{L}_y^2 + \hat{L}_z^2. \tag{6}$$

It is much easier to deal with this operator than it's square root. Fortunately, it is not necessary at this point to write $\hat{L}^2$ out in terms of elementary Cartesian component operators.

Can we expect general states in which the angular momentum components each (or even in pairs) take on precisely defined values? The answer is "no" as is shown by the non-zero value of the commutators of different components (we will find one counter example). For example,

$$[\hat{L}_x, \hat{L}_y] = [(\hat{y}\hat{p}_z - \hat{z}\hat{p}_y), (\hat{z}\hat{p}_x - \hat{x}\hat{p}_z)]. \tag{7}$$

This expands into four commutators, but only the diagonal terms (first times first, second times second) contain pairs of operators that do not commute; therefore, using the identities $[AB, C] = A[B, C] + [A, C]B$ and $[A, BC] = B[A, C] + [A, B]C$,

$$
\begin{aligned}
[\hat{L}_x, \hat{L}_y] &= [\hat{y}\hat{p}_z, \hat{z}\hat{p}_x] + [\hat{z}\hat{p}_y, \hat{x}\hat{p}_z] & (8)\\
&= \hat{y}[\hat{p}_z, \hat{z}\hat{p}_x] + [\hat{y}, \hat{z}\hat{p}_x]\hat{p}_z + \hat{z}[\hat{p}_y, \hat{x}\hat{p}_z] + [\hat{z}, \hat{x}\hat{p}_z]\hat{p}_y & (9)\\
&= \hat{y}[\hat{p}_z, \hat{z}\hat{p}_x] + 0 \qquad\quad + 0 \qquad\quad + [\hat{z}, \hat{x}\hat{p}_z]\hat{p}_y & (10)\\
&= \hat{y}[\hat{p}_z, \hat{z}]\hat{p}_x + \hat{y}\hat{z}[\hat{p}_z, \hat{p}_x] + [\hat{z}, \hat{x}]\hat{p}_z\hat{p}_y + \hat{x}[\hat{z}, \hat{p}_z]\hat{p}_y & (11)\\
&= \hat{y}[\hat{p}_z, \hat{z}]\hat{p}_x + 0 \qquad\quad + 0 \qquad\quad + \hat{x}[\hat{z}, \hat{p}_z]\hat{p}_y & (12)\\
&= i\hbar(\hat{x}\hat{p}_y - \hat{y}\hat{p}_x) = i\hbar\hat{L}_z. & (13)
\end{aligned}
$$

Working through the others yields

$$[\hat{L}_x, \hat{L}_y] = i\hbar\hat{L}_z \tag{14}$$

$$[\hat{L}_z, \hat{L}_x] = i\hbar\hat{L}_y \tag{15}$$

$$[\hat{L}_y, \hat{L}_z] = i\hbar\hat{L}_x. \tag{16}$$

In contrast to the above, the commutator $[\hat{L}^2, \hat{L}_i]$ is zero, so the magnitude and *one* component of **L** can be constant, precisely defined quantities. The proof is as follows for $\hat{L}_z$:

$$
\begin{aligned}
[\hat{L}^2, \hat{L}_z] &= [\hat{L}_x^2, \hat{L}_z] + [\hat{L}_y^2, \hat{L}_z] + [\hat{L}_z^2, \hat{L}_z] & (17)\\
&= [\hat{L}_x^2, \hat{L}_z] + [\hat{L}_y^2, \hat{L}_z] + 0 & (18)\\
&= \hat{L}_x[\hat{L}_x, \hat{L}_z] + [\hat{L}_x, \hat{L}_z]\hat{L}_x + \hat{L}_y[\hat{L}_y, \hat{L}_z] + [\hat{L}_y, \hat{L}_z]\hat{L}_y & (19)\\
&= \hat{L}_x(-i\hbar\hat{L}_y) + (-i\hbar)\hat{L}_y\hat{L}_x + \hat{L}_y(i\hbar\hat{L}_x) + (i\hbar\hat{L}_x)\hat{L}_y & (20)\\
&= 0. & (21)
\end{aligned}
$$

We conclude that it is possible to have states in which the magnitude and one component of the angular momentum are well-defined constants of the motion (in other words, in which the corresponding operators satisfy eigenvalue equations with the wavefunction that describes

the state).[1] However, not more than one component will, in general, satisfy this property in any given state. We will find functions that are eigenfunctions of $\hat{L}^2$ and $\hat{L}_x$ or $\hat{L}^2$ and $\hat{L}_y$ or $\hat{L}^2$ and $\hat{L}_z$ but these will not be eigenfunctions of, say, both $\hat{L}_z$ and $\hat{L}_x$. This situation implies that there exists more than one function with a given eigenvalue of $\hat{L}^2$. By convention, we will choose the z axis as the one that has an eigenvalue for its component. This is strictly a choice – no physical quantity should depend on our choice of coordinate system and, by the same token, we are free to orient our axes to put z in the "chosen" direction.

Total angular momentum.   Many systems have multiple "point masses" with each contributing to a total angular momentum. In fact, there are two types of contributions, one the classical orbital motion that we have just generalized to a quantum mechanical treatment, the other an intrinsic angular momentum or "spin" associated with the particle itself. The latter quantity has no classical analog but rather is a fundamental property of many types of elementary particles. We call it a "spin" angular momentum in spite of the fact that it cannot be explained in terms of a spinning sphere or any other classical picture.

We will refer to the two contributions as being orbital angular momentum, **L**, and spin angular momentum, **S**. When both contributions are present, we denote the total as $\mathbf{J} = \mathbf{L} + \mathbf{S}$. Keep in mind that in multiparticle systems, there may be several contributions to both **L** and **S**. It turns out (i.e., we guess and find out it's correct) that **J** obeys the same operator algebra as we derived above for **L**. For the rest of the derivation of quantum mechanical properties of angular momentum, we replace the **L**'s by **J**'s. Clearly, the proof of the appropriateness of this replacement is in experimental observations of the properties of systems having multiple contributors to **J**. Examples are as elementary as the hydrogen atom and as complex as magnetic and superconducting materials, stars,...

Note that a charged particle with orbital angular motion generates a magnetic dipole moment, $\mu = \frac{q}{2m}\mathbf{L}$; this is just the orbital current times the orbit area (as you can show for circular motion with elementary algebra – see also, Chapter 8). For electrons, we can write $\mu = -g\mu_B(\mathbf{J}/\hbar)$ with $\mu_B = \frac{e\hbar}{2m_e}$, with the factor g (called the g-factor, amazingly enough) accounting for the addition of orbital and spin contributions. μ_B is the *Bohr magneton* which sets the scale for magnetism generated by electrons (one can also define a *nuclear magneton*, μ_n, which is about 2000 times smaller). Note that $\mathbf{J}/\hbar$ is a dimensionless quantity. The orbital and spin angular momenta are intimately coupled to magnetic behavior and the response of atoms and materials and stars to magnetic fields. It is through the interaction of the magnetic moments with magnetic fields that most properties of the angular momenta are observed. *These elementary contributions, along with their interactions, yield all of magnetism!*

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[1]We have not tested whether the angular momentum operators commute with the Hamiltonian. Can states with well-defined L^2, L_z be energy eigenfunctions? We will find that the answer is yes only in the case of spherically symmetric potential energy functions – i.e., potentials that depend only or a radius, r, and not on the direction to the particle. Such potentials supply no torque to the particle since any force will be along the radial direction.

Angular momentum quantization. From the commutation relations discussed above, we conclude that we should be able to write

$$\hat{J}^2\psi = \alpha\psi \tag{22}$$
$$\hat{J}_z\psi = \beta\psi, \tag{23}$$

that is, there should be a wavefunction or wavefunctions, ψ, that satisfy these equations with particular eigenvalues, α and β. Note that these two eigenvalues do not have the same units.

It turns out to be very convenient to define two non-Hermitian operators, $\hat{\mathbf{J}}_+$ and $\hat{\mathbf{J}}_-$, called the raising and lowering operators – or, collectively, ladder operators (the terminology will be justified by their properties):

$$\hat{J}_+ = \hat{J}_x + i\hat{J}_y \tag{24}$$
$$\hat{J}_- = \hat{J}_x - i\hat{J}_y. \tag{25}$$

These are mutually adjoint rather than self-adjoint:

$$(\phi|\hat{J}_+\psi) = (\phi|(\hat{J}_x + i\hat{J}_y)\psi) \tag{26}$$
$$= (\phi|\hat{J}_x\psi) + (\phi|i\hat{J}_y\psi) \tag{27}$$
$$= (\hat{J}_x\phi|\psi) + (-i\hat{J}_y\phi|\psi) \tag{28}$$
$$= ((\hat{J}_x - i\hat{J}_y)\phi|\psi) = (\hat{J}_-\phi|\psi) \tag{29}$$

So, $\hat{J}_+^\dagger = \hat{J}_-$ and $\hat{J}_-^\dagger = \hat{J}_+$. Since these operators are non-Hermitian, they cannot correspond to a physically measurable quantity. However, they perform handy mathematical operations.

While the $\hat{J}_\pm$ commute with $\hat{J}^2$, they do not commute with component operators such as $\hat{J}_z$. First,

$$[\hat{J}^2, J_+] = [\hat{J}^2, \hat{J}_x] + i[\hat{J}^2, \hat{J}_y] = 0 \tag{30}$$
$$[\hat{J}_x, J_+] = [\hat{J}_x, \hat{J}_x] + i[\hat{J}_x, \hat{J}_y] = -\hbar\hat{J}_z \tag{31}$$
$$[\hat{J}_y, J_+] = [\hat{J}_y, \hat{J}_x] = -i\hbar\hat{J}_z \tag{32}$$
$$[\hat{J}_z, J_+] = i\hbar\hat{J}_y + \hbar\hat{J}_x = \hbar\hat{J}_+ \tag{33}$$

$\hat{J}_-$ yields the complex conjugates of these relations.

$\hat{J}_+$ and $\hat{J}_-$ are useful because when they operate on an angular momentum eigenfunction, they generate other ones (see Problem 5.10). For example, if $\hat{J}_+\psi = \phi$, then by using the commutation relation (30) and the definition of α (22),

$$\hat{J}^2\phi = \hat{J}^2(\hat{J}_+\psi) = \hat{J}_+\hat{J}^2\psi = \hat{J}_+\alpha\psi = \alpha\hat{J}_+\psi = \alpha\phi. \tag{34}$$

The new function, ϕ, has the same eigenvalue of $\hat{J}^2$. On the other hand, using (33) and (23),

$$\hat{J}_z\phi = \hat{J}_z(\hat{J}_+\psi) = (\hbar\hat{J}_+ + \hat{J}_+\hat{J}_z)\psi = (\hbar\phi + \hat{J}_+\beta\psi) = (\beta + \hbar)\phi. \tag{35}$$

So $\phi = \hat{J}_+\psi$ has an eigenvalue of $\hat{J}_z$ that is one unit of $\hbar$ larger than that of ψ. Similar calculations show that $\hat{J}_-$ maintains the same eigenvalue of $\hat{J}^2$ but an eigenvalue of $\hat{J}_z$

that is decreased by $\hbar$. These results justify the naming of these operators as "raising" and "lowering" operators. Classically, they rotate the angular momentum vector (of fixed length) so as to change the component that lies along the quantization axis, z.

Repeated operation with, say, $\hat{J}_+$ successively generates states with larger J_z but with the same $|J|$. However, there is the classically reasonable constraint that $\alpha \geq \beta^2$ (essentially saying that the z-component cannot be larger than the length of the whole vector). This can be seen more rigorously by calculating the expectation value of $\hat{J}^2$ and using (6). Bringing the J_z term to the left side and using the Hermitian property of the component operators,

$$(\psi|\hat{J}^2\psi) - (\psi|\hat{J}_z^2\psi) = (\psi|\hat{J}_x^2\psi) + (\psi|\hat{J}_y^2\psi) = (\hat{J}_x\psi|\hat{J}_x\psi) + (\hat{J}_y\psi|\hat{J}_y\psi) \tag{36}$$

The right side involves integrals of positive (or zero) functions and is therefore positive (or zero). The term $(\psi|\hat{J}_z^2\psi)$ is just β^2, so we have $\alpha - \beta^2 \geq 0$ or $\alpha \geq \beta^2$.

The result of the above paragraph implies that there must be some wavefunction, ψ_{max} that has the maximum possible eigenvalue, β_{max}, and that

$$\hat{J}_+\psi_{max} = 0. \tag{37}$$

Similarly, there must be a function, ψ_{min}, with the property

$$\hat{J}_-\psi_{min} = 0. \tag{38}$$

Two additional operators that will be used below are the products, $\hat{J}_-\hat{J}_+$ and $\hat{J}_+\hat{J}_-$:

$$\hat{J}_-\hat{J}_+ = (\hat{J}_x - i\hat{J}_y)(\hat{J}_x + i\hat{J}_y) = \hat{J}_x^2 + \hat{J}_y^2 + i[\hat{J}_x, \hat{J}_y] = \hat{J}^2 - \hat{J}_z^2 - \hbar\hat{J}_z \tag{39}$$

or

$$\begin{aligned}\hat{J}^2 &= \hat{J}_-\hat{J}_+ + \hat{J}_z^2 + \hbar\hat{J}_z \tag{40}\\ &= \hat{J}_+\hat{J}_- + \hat{J}_z^2 - \hbar\hat{J}_z \tag{41}\end{aligned}$$

Operating with $\hat{J}^2$ in the form of (40) on ψ_{max} yields

$$\hat{J}^2\psi_{max} = \alpha\psi_{max} = 0 + \beta_{max}^2\psi_{max} + \hbar\beta_{max}\psi_{max} \tag{42}$$

or

$$\alpha = \beta_{max}(\beta_{max} + \hbar). \tag{43}$$

Using (41) on ψ_{min} yields

$$\alpha = \beta_{min}(\beta_{min} - \hbar). \tag{44}$$

Subtracting these two yields $\beta_{max}(\beta_{max} + \hbar) = \beta_{min}(\beta_{min} - \hbar)$ which is satisfied by $\beta_{min} = -\beta_{max}$.

Furthermore, if we start at β_{min}, we can write $\beta_{max} = \beta_{min} + n\hbar$ for some integer, n. Replacing β_{min} with $-\beta_{max}$ leads to

$$2\beta_{max} = n\hbar \tag{45}$$

or

$$\beta_{max} = \frac{n}{2}\hbar. \tag{46}$$

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This in turn leads to

$$\alpha = \beta_{max}(\beta_{max} + \hbar) = \frac{n}{2}(\frac{n}{2} + 1)\hbar^2. \tag{47}$$

Defining $j = \frac{n}{2} = 0, \frac{1}{2}, 1, \frac{3}{2}, 2, ...$, leads to the condition that the set of possible eigenvalues of $\hat{J}^2$ can be written as

$$\boxed{J^2 = j(j + 1)\hbar^2 \text{ with } j = 0, \frac{1}{2}, 1, \frac{3}{2}, 2, ...} \tag{48}$$

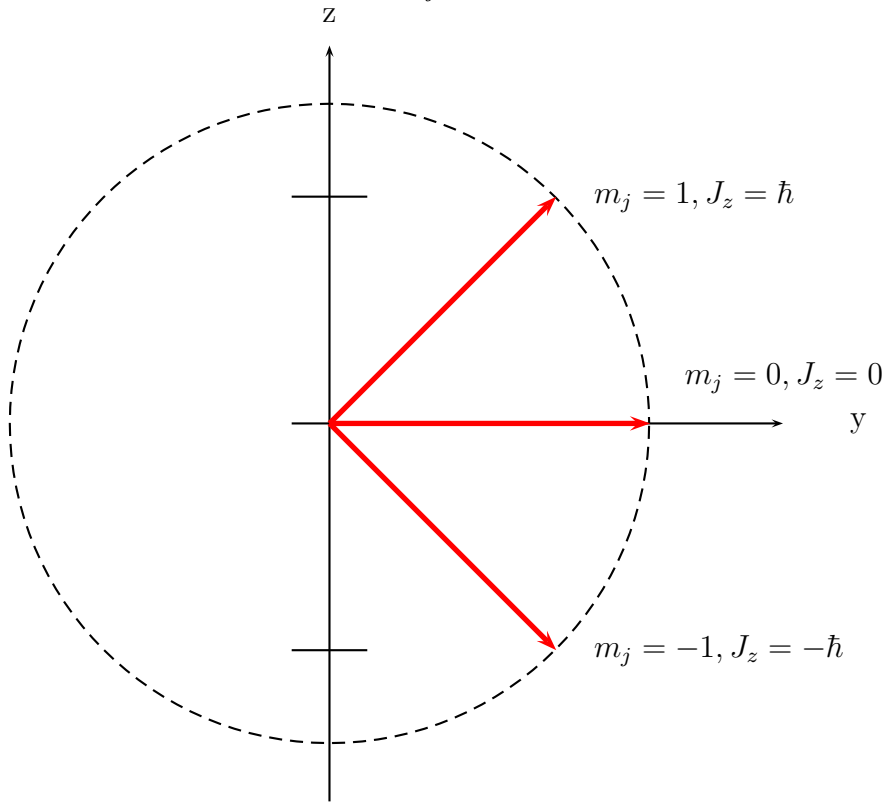and the eigenvalues of $\hat{J}_z$, for a given j, must be one of these:

$$\boxed{J_z = m_j\hbar, \ m_j = -j, (-j + 1), ..., (j - 1), j.} \tag{49}$$

The language is that j is called the "angular momentum quantum number" and m_j is the "azimuthal quantum number." j gives the magnitude (or length) of the vector $\mathbf{J}$, and m_j gives the component of this vector along the z-axis. In all cases, the eigenvalues satisfy $J^2 > J_z^2$. The classical limit is obtained as $j \to \infty$ where the relative spacing between values of J^2 becomes negligible and the component values, J_z, become essentially continuous.
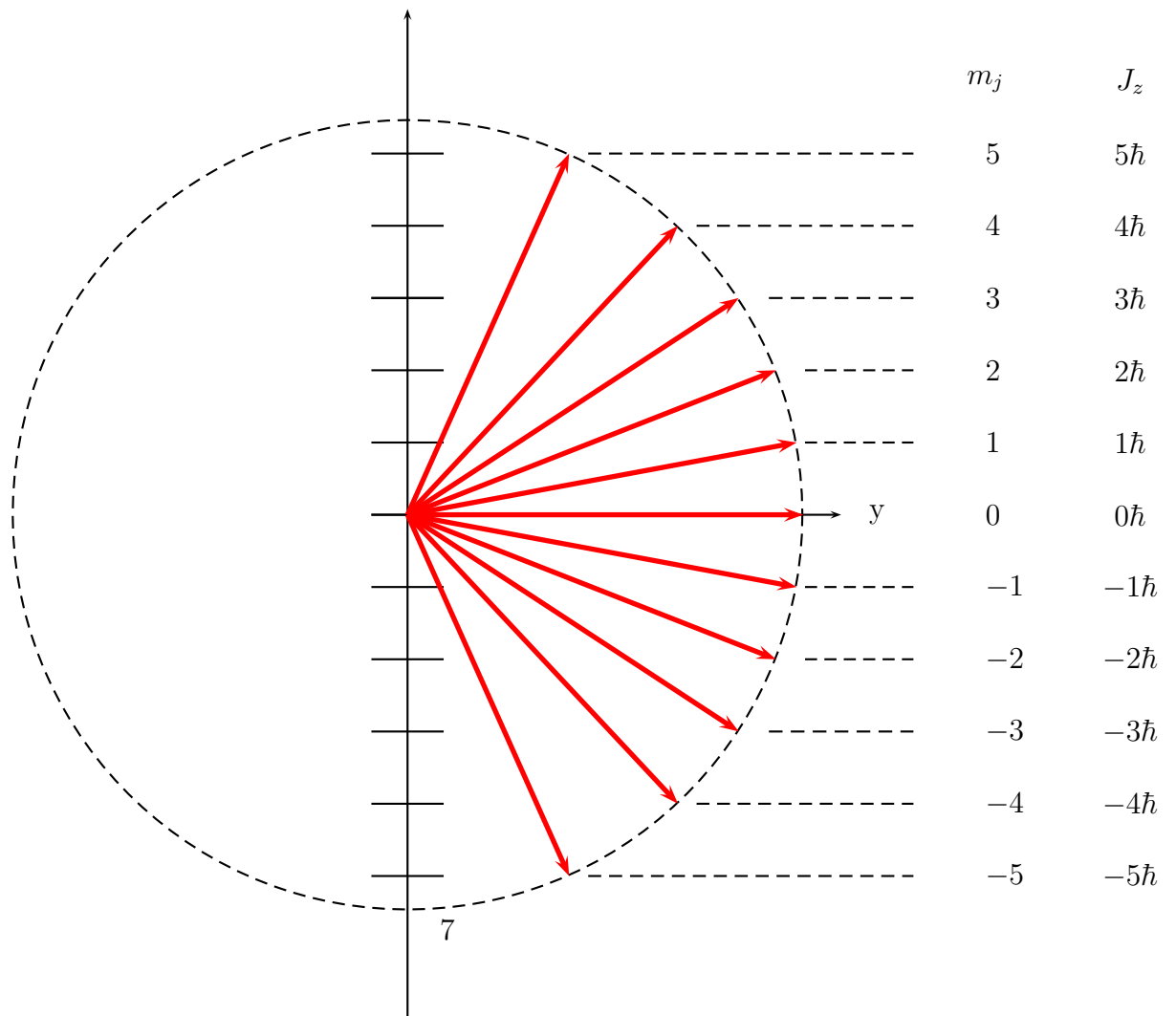
Final note: We have not written down any explicit wavefunctions in the above derivation. While this makes the derivation rather abstract, it also emphasizes the generality of the arguments: the results above are the properties of angular momentum that are allowed by quantum mechanics – for any system! They are also the properties that are observed in the real world. While the existence of spin angular momentum is a relativistic effect, the behavior of all particles and collections of particles can be understood with the above results plus some rules for how to add angular momenta in composite systems so as to preserve the above behavior for the total angular momentum.

The following page shows drawings for two examples of the quantization rules we have just derived: these are appropriate for orbital angular momenta with $l_1 = 1$ and $l_2 = 5$. The scales are NOT the same for the two drawings; if they were, then the second circle would be larger by a factor of $\frac{\sqrt{l_2(l_2+1)}\hbar}{\sqrt{l_1(l_1+1)}\hbar} = \frac{\sqrt{30}}{\sqrt{2}} = \sqrt{15} = 3.873$ and the spacings between the marks on the z-axis would be equal in the two pictures.

Example 1: $j = 1$ allows $m_j = -1, 0, +1$

z

$m_j = 1, J_z = \hbar$

$m_j = 0, J_z = 0$

y

$m_j = -1, J_z = -\hbar$

Example 2: $j = 5$ allows $m_j = -5, -4, -3, -2, -1, 0, 1, 2, 3, 4, 5$

z

m_j	J_z
5	$5\hbar$
4	$4\hbar$
3	$3\hbar$
2	$2\hbar$
1	$1\hbar$
0	$0\hbar$
-1	$-1\hbar$
-2	$-2\hbar$
-3	$-3\hbar$
-4	$-4\hbar$
-5	$-5\hbar$

y

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Many elementary particles (electrons, muons, taus, neutrinos, quarks, lambdas...) as well as protons and neutrons (which are composite particles) have spin quantum number $S = 1/2$. These particles can have only two distinct projections onto a measurement axis. Pions, Kons and the Higgs particle have spin zero so they carry no angular momentum. The omega particle has spin $3/2$.

Magnetic properties of materials are determined by the combined effects of orbital and spin angular momenta of the atomic electrons. We will discuss this after solving the hydrogen atom problem.

In conclusion, we find that only a discrete (but infinite) set of values are possible for either the total angular momentum magnitude or for the component of angular momentum along a particular direction. For a finite magnitude only a finite discrete set of components occur. Classically, this corresponds to a finite set of angular momentum vector orientations relative to some coordinate axis. Note that, as $j \to \infty$, the set of possible components becomes infinite and the quantum description becomes similar to the classical picture in which all orientations are possible.

Again, so far, we have not tried to write down any wavefunctions other than symbolically (i.e., ψ or ϕ). We will find that we can do this for the orbital motion of a particle in a spherically symmetric potential but that we only obtain functions for integer values: $l = 0, 1, 2, ...$ with corresponding integer azimuthal quantum numbers, m_l (l and m_l are used here to explicitly show that these are components of orbital motion as distinct from the intrinsic angular momentum of elementary particles). Elementary particles can have half-integer quantum numbers for their "spin" angular momenta, s and m_s. In this case, there is no function of spatial variables that describes these properties; we will have to develop another means to represent operators for these degrees of freedom. Nevertheless, the spin eigenstates are described by the same rules we have just developed.

For particles with spin angular momentum undergoing orbital motion, we will have to learn how to add the orbital and spin contributions to obtain total angular momenta with quantum numbers, j and m_j. Furthermore, collective properties of quantum particles differ profoundly depending on the spin quantum number: particles with integer spin quantum number, s, called bosons, behave dramatically differently from half-integer spin particles called Fermions. Bosons can undergo condensation into a single quantum state, while Fermions obey the Pauli exclusion principle with no more than one being in a given quantum state. This is a phenomenon with no classical limit or correspondence!

Strictly speaking, we have not derived anything but the results of applying $\hat{J}_+$ and $\hat{J}_-$ to the orbital angular momentum operators guessed from classical mechanics. You might say that we have simply come up with a way to enumerate the quantum states associated with angular momentum. The states we obtain here are, in fact, those that occur in nature; no other states have ever been observed!