PHYS 500 (Quantum Mechanics I) Notes

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Introduction:

This is a set of lecture notes taken from UBC's PHYS 500 (Graduate Quantum Mechanics I) course, taught by Dr. Ariel Zhinitsky. The course covers Angular momentum and spin, electromagnetic interactions, Time-independent perturbation theory, the WKB approximation, Time-dependent perturbation theory, the adiabatic approximation, and scattering. If any errors are found in the notes, feel free to email me at ryoheiweil@phas.ubc.ca.

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1 Angular Momentum

1.1 Units

We set $\hbar = 1$ for this course (natural units), unless we are doing a numerical estimate of some quantity.

1.2 Angular Momentum - Definitions

Angular momentum operators obey the commutation relations:

$$[L_i, L_j] = i\epsilon_{ijk} L_k. \tag{1.1}$$

Where ϵ_{ijk} is the Levi-Cicata symbol, defined as:

$$\epsilon_{ijk} = \begin{cases} +1 & ijk \text{ is an even permutation of } 123 \\ -1 & ijk \text{ is an odd permutation of } 123 \\ 0 & \text{otherwise} \end{cases} \tag{1.2}$$

We also follow the Einstein summation convention, where repeated indices are implicitly summed over. We also define the raising/lowering operators:

$$L_\pm = L_x \pm iL_y \tag{1.3}$$

and the total angular momentum:

$$\mathbf{L}^2 = L_x^2 + L_y^2 + L_z^2. \tag{1.4}$$

It can be easily verified that:

$$[\mathbf{L}^2, L_i] = 0 \tag{1.5}$$

and that:

$$[L_z, L_+] = [L_z, L_x + iL_y] = +L_+ \tag{1.6}$$

$$[L_z, L_-] = -L_- \tag{1.7}$$

$$[\mathbf{L}^2, L_\pm] = 0 \tag{1.8}$$

Note that while L_i are Hermitian operators (they are observables), the $L_\pm$ are not (this can be verified by the definition of the Hermitian conjugate). However this does not mean that it is not useful. Now, we ask, what is the physical meaning of:

$$[\mathbf{L}^2, L_z] = 0 \tag{1.9}$$

The answer is that we can know/measure $\mathbf{L}^2$ and L_z simultaneously. Next, what is the meaning of:

$$[\mathbf{L}^2, L_\pm] = 0 \tag{1.10}$$

This means that if we apply $L_\pm$ to an eigenstate of $\mathbf{L}^2$, we do not change the eigenstate. Now, what is the physical meaning of:

$$[L_z, L_+] = L_+? \tag{1.11}$$

It tells us that L_+ is a raising operator for L_z; it increments the eigenvalue of L_z.

1.3 Angular Momentum - Eigenvalues

Let us now proceed with our construction. Consider the simultaneous eigenbasis of $\mathbf{L}^2$ and L_z. Let us call the kets of this eigenbasis as $|l, m\rangle$. We want to solve the eigenvalue problem:

$$\begin{aligned} \mathbf{L}^2|l,m\rangle &= \lambda|l,m\rangle. \\ L_z|l,m\rangle &= m|l,m\rangle \end{aligned} \tag{1.12}$$

Let us back up for a moment; why can we define a simultaneous eigenbasis? Of course this follows from the fact that $\mathbf{L}^2$ and L_z commute:

$$[\mathbf{L}^2, L_z] = 0 \implies [\mathbf{L}^2, L_z]|l,m\rangle = 0. \tag{1.13}$$

Let us also check our physical interpretation of L_+. We know that $L_+|l,m\rangle$ should give us another eigenstate of $\mathbf{L}^2$ and L_z (which we can call $|x\rangle$), but to this end we calculate:

$$[\mathbf{L}^2, L_\pm] = 0 \implies [\mathbf{L}^2, L_\pm]|l,m\rangle = 0. \tag{1.14}$$

so we know that:

$$\mathbf{L}^2|x\rangle - \lambda|x\rangle = 0. \tag{1.15}$$

Now, we know that $[L_z, L_+] = L_+$, so:

$$[L_z, L_+]|l,m\rangle = L_+|l,m\rangle. \tag{1.16}$$

Expanding the above, we have:

$$L_z|x\rangle - m|x\rangle = |x\rangle. \tag{1.17}$$

So rearranging we have:

$$L_z|x\rangle = (m+1)|x\rangle \tag{1.18}$$

And we can find an analogous result for L_-. We don't yet know how to normalize these states (we will do so later). But the above result is purely algebraic; no differential equations or spherical harmonics to be found. Let us continue and find the eigenvalues in an algebraic manner. If we recall the definition of $\mathbf{L}^2$ in Eq. (1.4), we have:

$$\mathbf{L}^2 = L_z^2 + L_y^2 + L_x^2 = L_z^2 + (L_x + iL_y)(L_x - iL_y) + i(L_xL_y - L_yL_x). \tag{1.19}$$

Now using what we know of the angular momentum commutation relations and the raising/lowering operators:

$$\mathbf{L}^2 = L_z^2 + L_+L_- - L_z = L_z^2 + L_-L_+ + L_z \tag{1.20}$$

Now, we consider applying the lowering operator L_- many many times. We then get to a state with the lowest projection m_{min}. We then have that:

$$L_-|l, m_{min}\rangle = 0. \tag{1.21}$$

This arises from the fact that we cannot decrease m further than the total angular momentum value (much in the same way that we cannot go below the ground state of the quantum harmonic oscillator). Analogously, we have:

$$L_+|l, m_{max}\rangle = 0. \tag{1.22}$$

Now, we apply $\mathbf{L}^2$ to the minimum projection eigenstate. Then using the form of $\mathbf{L}^2$ derived above, we have:

$$\mathbf{L}^2|l, m_{min}\rangle = (L_z^2 + L_+L_- - L_z)|l, m_{min}\rangle = (L_z^2 - L_z)|l, m_{min}\rangle = (m_{min}^2 - m_{min})|l, m_{min}\rangle \tag{1.23}$$

and analogously:

$$\mathbf{L}^2|l, m_{max}\rangle = (L_z^2 + L_-L_+ + L_z)|l, m_{max}\rangle = (L_z^2 + L_z)|l, m_{max}\rangle = (m_{max}^2 + m_{max})|l, m_{max}\rangle. \tag{1.24}$$

From this we obtain that:

$$(m_{min}^2 - m_{min}) = (m_{max}^2 + m_{max}) \tag{1.25}$$

as the magnitude/eigenvalue of $\mathbf{L}^2$ on the min/max projections should be the same. The above equation only has one nontrivial solution:

$$m_{max} = -m_{min}. \tag{1.26}$$

Now, we observe that we have an integer number of steps (as L_+/L_- raise/lower by integers), so:

$$m_{max} - m_{min} = N \in \mathbb{N} \tag{1.27}$$

And therefore:

$$2m_{max} = N \implies m_{max} = \frac{N}{2}. \tag{1.28}$$

That is to say that the eigenvalues of angular momentum can be integers or half-integers. We can conclude the eigenvalue relations:

$$\mathbf{L}^2|l, m\rangle = l(l+1)|l, m\rangle \tag{1.29}$$

$$L_z|l, m\rangle = m|l, m\rangle \tag{1.30}$$

where l or m are either integers or half integers.

Now, we move onto the question of degeneracy. We have a $2l + 1$ degeneracy, where we count:

$$m = -l, -l+1, \ldots, 0, \ldots, l-1, l. \tag{1.31}$$

Now, we suppose we want to compute $\langle l, m|L_x|l, m\rangle$. It turns out to be zero, but how do we show this? Physically, we can say that L_x is completely uncorrelated with L_z and so we should get zero. Mathematically we can use ladder operators:

$$\langle l, m|L_x|l, m\rangle = \langle l, m|L_+ + L_-|l, m\rangle = \langle l, m|\left(|l, m+1\rangle + |l, m-1\rangle\right)0 \tag{1.32}$$

where in the last relation we use that the $|l, m\rangle$ are orthogonal. Now we ask what about $\langle l, m|L_x^2|l, m\rangle$? It is nonzero. We can calculate this by:

$$\langle l, m|L_x^2|l, m\rangle = \langle l, m|\mathbf{L}^2 - L_z^2 - L_y^2|l, m\rangle \tag{1.33}$$

by symmetry we can conclude that $\langle l, m|L_x^2|l, m\rangle = \langle l, m|L_y^2|l, m\rangle$, and so:

$$\langle l, m|L_x^2|l, m\rangle = \frac{1}{2}\langle l, m|(\mathbf{L}^2 - L_z^2)|l, m\rangle = \frac{1}{2}\left[l(l+1) - m^2\right]. \tag{1.34}$$

2 Angular Momentum, Continued

2.1 Review of Lecture 1

We start by reviewing the important points of last class. Using the commutation relations for $\mathbf{L}^2, L_z, L_\pm$, we established that $L_\pm$ do not change the eigenvalue of $\mathbf{L}^2$ when acting on an joint eigenstate of $\mathbf{L}^2/L_z$, and we established the equations:

$$\mathbf{L}^2 = L_z^2 + L_\pm L_\mp \mp L_z. \tag{2.1}$$

$\mathbf{L}^2$ is the same for the highest and lowest states for L_z, and we established that $m_{max} = -m_{min}$. We found that the eigenvalues of L_z jump in integer steps, and can take either integer or half-integer values. The main point is that we derived this purely algebraically (we did not solve Legendre polynomials). Note that

$$L_+|l, m_{max}\rangle = L_-|l, m_{min}\rangle = 0 \tag{2.2}$$

is equivalent to the boundary conditions when solving this problem in the differential equations approach. We found that:

$$\langle l, m|L_\pm|l, m\rangle = 0. \tag{2.3}$$

by orthogonality, and using that $L_{x/y} = (L_+ \pm L_-)/2$ that:

$$\langle l, m|L_{x/y}|l, m\rangle = \langle l, m|\frac{L_+ + L_-}{2}|l, m\rangle = 0. \tag{2.4}$$

2.2 Parity and Pseudovectors

It is clear that:

$$\langle l, m|L_z|l, m\rangle = m. \tag{2.5}$$

We now ask, what is the value of $\langle l, m|Z|l, m\rangle$ and $\langle l, m|X|l, m\rangle$? We find that:

$$\langle l, m|Z|l, m\rangle = \langle l, m|X|l, m\rangle = 0 \tag{2.6}$$

as when we specify the angular momentum, we know nothing of the position.

How would we do this rigorously? We will come back to this when we do selection rules. For now, let us consider defining the parity operator P that takes a vector $\mathbf{v}$ and maps it to $-\mathbf{v}$. So, each of the position operators get mapped to their negative (i.e. $P^\dagger X P = -X$). Using this in tandem with the fact that $|l, m\rangle$ are eigenvalues of parity (with eigenvalues $(-1)^l$, as we will discuss below), we could conclude that the above expectation values vanish, as:

$$\langle l, m|X|l, m\rangle = \langle l, m|(-1)^l X(-1)^l|l, m\rangle = \langle l, m|P^\dagger X P|l, m\rangle = \langle l, m|(-X)|l, m\rangle = -\langle l, m|X|l, m\rangle \tag{2.7}$$

and comparing the first and last expressions we find that the expectation value is zero. However, we may then ask why does the expectation value of L_z not vanish? This is because angular momentum (like torque and magnetic fields) are not vectors, but rather pseudovectors.

2.3 Parity Spherical harmonics

Let us take a closer look at how parity is related to eigenkets of angular momentum. In the position basis, we can write them as spherical harmonics:

$$|l, m\rangle \cong Y_l^m(\theta, \varphi). \tag{2.8}$$

Consider a unit vector in 3d:

$$\hat{n} = (n_x, n_y, n_z) = (\sin\theta\cos\varphi, \sin\theta\sin\varphi, \cos\theta). \tag{2.9}$$

How do the spherical harmonics behave under $Y_l^m(\hat{n}) \to Y_l^m(-\hat{n})$ (in terms of angles, $\theta \to \pi - \theta, \varphi \to \varphi + \pi$) They transform as:

$$Y_l^m(-\hat{n}) = (-1)^l Y_l^m(\hat{n}). \tag{2.10}$$

Let us look at a couple examples. $Y_0^0 \sim \frac{1}{\sqrt{4\pi}}$ so is unchanged under the flip of the vector. $Y_1^0 \sim \cos\theta$ so this maps to $\cos(-\theta) \to -\cos\theta$ under a flip of the vector. $Y_1^1 \sim \sin\theta e^{i\varphi}$, so the $\sin\theta$ stays the same under interchange but $e^{i\varphi}$ flips sign so it maps to $-Y_1^1$.

Note this discussion is really trying to motivate the use of symmetry to skip doing computations; we don't have to compute integrals if we know the symmetry of the system.

Another example (returning to the above discussion of expectation values of position). Hopefully by now we would be convinced that:

$$\langle l, m|\mathbf{R}|l, m\rangle = 0. \tag{2.11}$$

by the above arguments showing that $|l, m\rangle$ are eigenvalues of parity with eigenvalue $(-1)^l$. Now what about $\langle l+1, m|\mathbf{R}|l, m\rangle$? In this case it is *nonzero* as the negative signs cancel when we consider the parity properties.

2.4 Eigenvalues of Ladder Operators

We know that the ladder operators follow the relation:

$$L_+|l, m\rangle = c_+|l, m+1\rangle \tag{2.12}$$

but we have yet to calculate c_+. Let us do this now. We consider acting L_- on the dual of $|l, m\rangle$:

$$\langle l, m|L_- = c_+^*\langle l, m+1| \tag{2.13}$$

So therefore:

$$\langle l, m|L_-L_+|l, m\rangle = |c_+|^2\langle l, m+1|l, m+1\rangle \tag{2.14}$$

so:

$$|c_+|^2\langle l, m|\mathbf{L}^2 - L_z^2 - L_z|l, m\rangle = l(l+1) - m^2 - m \tag{2.15}$$

so we conclude:

$$c_+ = \sqrt{l(l+1) - m(m+1)} \tag{2.16}$$

and an analogous computation can be done to find c_-.

2.5 Spin 1/2

Because of the degeneracy of angular momentum $(2l+1)$ derived via the Schrodinger equation, people expected to always see an odd number of lines when (e.g.) measuring the energy lines of atoms. But this turned out not to be true in experimental results; this is because not only does angular momentum come in orbital form, but also in an intrinsic form known as spin. This formalism and theory was developed by Pauli, and we now begin to explore it here through discussion of spin-1/2 systems. For such systems, we have $s = 1/2$, where the spin operators follow the commutation relations:

$$[S_i, S_j] = i\epsilon_{ijk}S_k. \tag{2.17}$$

Since there are $(2s+1)$ states, we have only two spin eigenstates:

$$|s = \frac{1}{2}, s_z = +\frac{1}{2}\rangle, |s = \frac{1}{2}, s_z = -\frac{1}{2}\rangle \tag{2.18}$$

Which obey:

$$S_+|s=\frac{1}{2},s_z=+\frac{1}{2}\rangle=0, S_-|s=\frac{1}{2},s_z=-\frac{1}{2}\rangle=0 \tag{2.19}$$

Given this, a natural notation for these states is:

$$|\uparrow\rangle \coloneqq |s=\frac{1}{2},s_z=+\frac{1}{2}\rangle, |\downarrow\rangle \coloneqq |s=\frac{1}{2},s_z=-\frac{1}{2}\rangle \tag{2.20}$$

So the above relations become (e.g.) $S_+|\uparrow\rangle = 0$. The total spin operator is given by:

$$\mathbf{S} \cong \frac{1}{2}\boldsymbol{\sigma} \tag{2.21}$$

where $\boldsymbol{\sigma} = (\sigma_x, \sigma_y, \sigma_z)^T$, with the Pauli matrices given by:

$$\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}. \tag{2.22}$$

Note that there is no reference to coordinates whatsoever here; everything is purely algebraic. Now, what is the value of $\mathbf{S}^2|\uparrow\rangle$? From the theory of angular momentum, we know that:

$$\mathbf{S}^2|\uparrow\rangle = s(s+1)|\uparrow\rangle = \frac{3}{4}|\uparrow\rangle. \tag{2.23}$$

But let us derive this result using the matrix form of $\mathbf{S}^2$. We can explicitly calculate to find that:

$$\sigma_i^2 = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \tag{2.24}$$

for each of the pauli matrices, so:

$$\mathbf{S}^2 \cong \frac{1}{4}(\sigma_x^2+\sigma_y^2+\sigma_z^2) = \frac{3}{4}\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}. \tag{2.25}$$

So with the choice of representation that $|\uparrow\rangle \cong \begin{pmatrix} 1 \\ 0 \end{pmatrix}$ and $|\downarrow\rangle \cong \begin{pmatrix} 0 \\ 1 \end{pmatrix}$, we find:

$$\mathbf{S}^2|\uparrow\rangle = \frac{3}{4}|\uparrow\rangle, \tag{2.26}$$

along with:

$$S_z|\uparrow\rangle = |\uparrow\rangle. \tag{2.27}$$

by looking at these matrix expressions. From now on, we will focus on spin-1/2 (though we will explore spin-1 in the homework). We will discuss the most general spin 1/2 state. It is given by:

$$|\chi\rangle = c_+|\uparrow\rangle + c_-|\downarrow\rangle. \tag{2.28}$$

In the spinor representation, it is given by:

$$\chi = \begin{pmatrix} c_+ \\ c_- \end{pmatrix}. \tag{2.29}$$

How many real parameters are needed to specify the quantum state? Naively, we would say 4 (2 complex numbers). But it turns out to be only two. One parameter is reduced by the normalization condition:

$$|c_+|^2 + |c_-|^2 = 1. \tag{2.30}$$

We also have a reduction of one from the fact that the state is physically unchanged when multiplied by a global phase $|\chi\rangle \sim e^{i\varphi}|\chi\rangle$; this comes from the fact that we can only measure probabilities in QM, and when we calculate these (using the Born rule, $p(i) = \langle\psi|\Pi_i|\psi\rangle$ the global phase cancells out). An important distinction: *relative* phases are observable (e.g. in neutron inferometry experiments), while global ones are not. So in the case of a single spin-1/2 particle, we can neglect the phase, but when we have multiple particles we cannot neglect relative phases.

2.6 Magnetic Hamiltonians

Consider the Hamiltonian:

$$\mathcal{H} = -\boldsymbol{\mu} \cdot \mathbf{B}. \tag{2.31}$$

where $\boldsymbol{\mu} = \gamma \boldsymbol{s}$ is the magnetic moment; we have an interaction between an external magnetic field $\mathbf{B}$ and the spin of a quantum particle. Note that the γ coefficient in the magnetic moment cannot be estimated by classical physics; a full calculation requires considering the Dirac field in QFT. But it can also be measured via experiment.

Next time, we will continue our discussion of this Hamiltonian and the evolution of spin states under it. We will also discuss Gauge invariance in the context of quantum mechanics.