Quantum Mechanics (P304H)
Part 2 – Lecture 15

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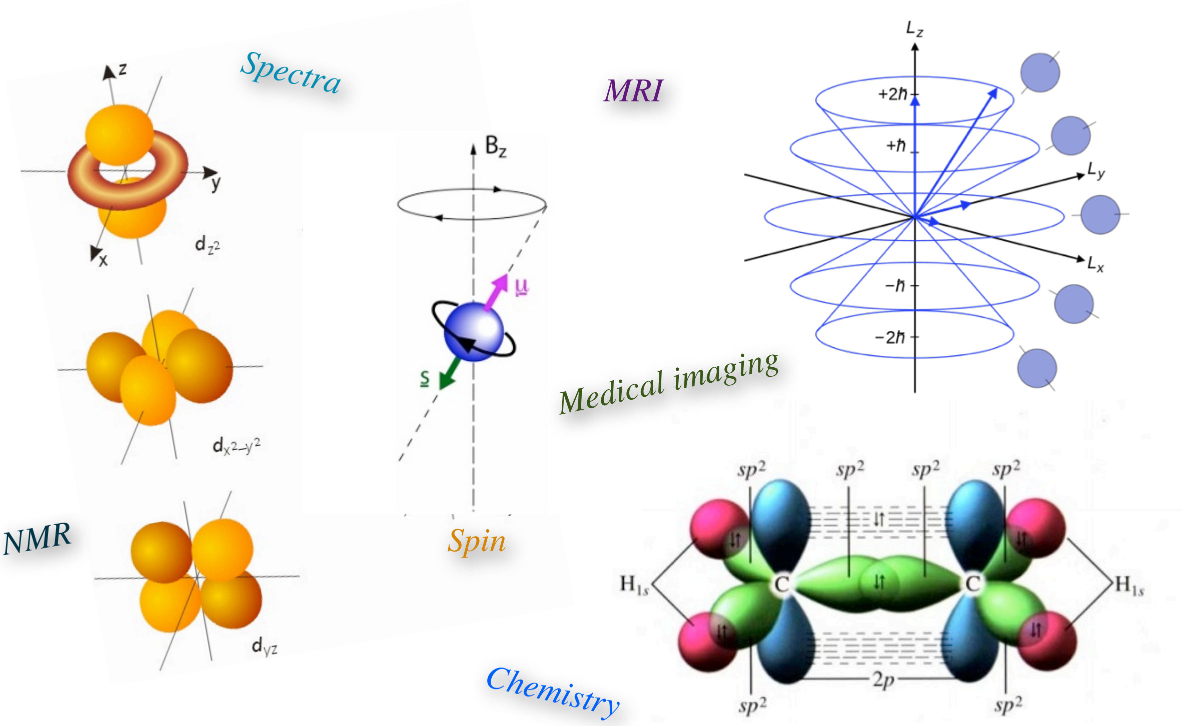
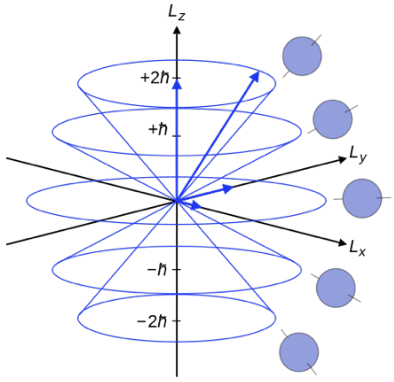
Switching to 3D: Angular Momentum



8. Angular Momentum

– Angular momentum is important and used in many domains of physics to describe atomic, molecular and nuclear spectra, the spin of elementary particles, magnetism, etc.
– Classically, it is a *constant of motion*, *i.e.* a conserved quantity in an isolated system
– In a central potential $dL/dt=0$
– There are also typical QM angular momenta with no classical equivalents
– Stern-Gerlach experiment
– Zeeman effect and applications: NMR, magnetic resonance imaging (MRI) and Mössbauer spectroscopy
– General QM properties of angular momenta follow from commutation relations between the associated operators



Notations:

L - *orbital* (with classical equivalent)

S - *spin* (with no classical equivalent)

J - *total* ($J=L+S$) or any arbitrary angular momentum

8. Operators recap

❑ Review of commutation relations for operators:

– The commutator was defined as: $\left[\hat{A},\hat{B}\right]=\hat{A}\hat{B}-\hat{B}\hat{A}$

In general, for operators in QM: $\left[\hat{A},\hat{B}\right]\neq 0$ (non-Abelian algebra)

– Momentum and position operators do not commute:

$$\left[\hat{x},\hat{p}_x\right]=i\hbar \quad \text{with} \quad \hat{x}=x \quad \text{and} \quad \hat{p}_x=(-i\hbar)\frac{d}{dx}$$

(Shown in QM Part 1)

– Commutator algebra reminders:

$$1)\left[\hat{A},\hat{B}\right]=-\left[\hat{B},\hat{A}\right];$$

$$2)\left[\alpha\hat{A},\beta\hat{B}\right]=\alpha\beta\left[\hat{A},\hat{B}\right];$$

$$3)\left[\hat{A},\hat{B}\pm\hat{C}\right]=\left[\hat{A},\hat{B}\right]\pm\left[\hat{A},\hat{C}\right]$$

$$4)\left[\hat{A},\hat{B}\hat{C}\right]=\left[\hat{A},\hat{B}\right]\hat{C}+\hat{B}\left[\hat{A},\hat{C}\right];$$

$$5)\left[\hat{A},\left[\hat{B},\hat{C}\right]\right]+\left[\hat{B},\left[\hat{C},\hat{A}\right]\right]+\left[\hat{C},\left[\hat{A},\hat{B}\right]\right]=0$$

8. Hermitian operators

- Quantum mechanical operators are Hermitian, i.e.

$$\int_{-\infty}^{\infty} \psi^*(x)\left(\hat{Q}\varphi(x)\right)dx = \int_{-\infty}^{\infty} \left(\hat{Q}\psi\right)^* \varphi(x)dx$$

Eigenvalues of Hermitian operators are real. Proof:

$$\hat{Q}\varphi(x) = q\varphi(x) \Rightarrow$$

$$\int_{-\infty}^{\infty} \varphi^*(x)\left(\hat{Q}\varphi(x)\right)dx = \int_{-\infty}^{\infty} \varphi^*(x)\left(q\varphi(x)\right)dx = q\int_{-\infty}^{\infty} \varphi^*(x)\varphi(x)dx = q$$

$$\int_{-\infty}^{\infty} \left(\hat{Q}\varphi(x)\right)^* \varphi(x)dx = \int_{-\infty}^{\infty} \left(q\varphi(x)\right)^* \varphi(x)dx = q^*\int_{-\infty}^{\infty} \varphi^*(x)\varphi(x)dx = q^*$$

$$q = q^* \Leftrightarrow q \in \mathbb{R}$$

8. Compatible observables

- A complete set of commuting observables is a set of commuting operators whose eigenvalues completely specify the state of a system.
- If there exists a complete set of functions ψ_n, such that each function is an eigenfunction of two operators $\hat{A}$ and B, then the observables of the operators are said to be compatible.

$$\begin{aligned} \hat{A}\psi_n &= a_n\psi_n \\ \hat{B}\psi_n &= b_n\psi_n \end{aligned} \quad \Rightarrow \hat{A}\hat{B}\psi_n = \hat{A}b_n\psi_n = a_n b_n\psi_n = b_n a_n\psi_n = \hat{B}\hat{A}\psi_n$$

Two compatible observables commute!

- If A and B commute, the measurement of one observable has no effect on the result of measuring the other.
- In Quantum Mechanics the only measurements that can be performed simultaneously are those of operators that commute. The Heisenberg uncertainty relation arises because the momentum and position operators cannot be measured simultaneously, since their operators do not commute.

8. Angular Momentum

- In Quantum Mechanics, angular momentum is a fundamental concept. Let us introduce it step by step.
- Orbital angular momentum is defined as:
  - In classical mechanics: $\underline{L} = \underline{r} \times \underline{p} \Rightarrow \quad L = rp\sin\alpha$

$$\underline{L} = \begin{vmatrix} \underline{i} & \underline{j} & \underline{k} \\ x & y & z \\ p_x & p_y & p_z \end{vmatrix} \Rightarrow \begin{cases} L_x = yp_z - zp_y \\ L_y = zp_x - xp_z \\ L_z = xp_y - yp_x \end{cases}$$

The underline is used as vector symbol here

  - In Quantum Mechanics, we substitute the operators:

$$\hat{\underline{r}} = (\hat{x}, \hat{y}, \hat{z})$$

$$\hat{\underline{p}} = (\hat{p}_x, \hat{p}_y, \hat{p}_z) = (-i\hbar)\left(\frac{\partial}{\partial x}, \frac{\partial}{\partial y}, \frac{\partial}{\partial z}\right) \Rightarrow$$

$$\hat{L}_x = -i\hbar\left(y\frac{\partial}{\partial z} - z\frac{\partial}{\partial y}\right)$$
$$\hat{L}_y = -i\hbar\left(z\frac{\partial}{\partial x} - x\frac{\partial}{\partial z}\right)$$
$$\hat{L}_z = -i\hbar\left(x\frac{\partial}{\partial y} - y\frac{\partial}{\partial x}\right)$$

8. Angular Momentum

- The orbital angular momentum operator is then:

$$\hat{\underline{L}} = -i\hbar(\underline{r} \times \underline{\nabla}) \qquad \text{where} \qquad \underline{\nabla} = \left(\frac{\partial}{\partial x}, \frac{\partial}{\partial y}, \frac{\partial}{\partial z}\right)$$

The angular momentum operator is Hermitian, since $\underline{r}$ and $\underline{p}$ are Hermitian.

- Commutation relations:
  - Since $[\hat{x}, \hat{p}_x] = [\hat{y}, \hat{p}_y] = [\hat{z}, \hat{p}_z] = i\hbar$ and

$$[\hat{x}, \hat{p}_y] = [\hat{x}, \hat{p}_z] = [\hat{y}, \hat{p}_x] = [\hat{y}, \hat{p}_z] = [\hat{z}, \hat{p}_x] = [\hat{z}, \hat{p}_y] = 0$$

we get $[\hat{x}, \hat{L}_x] = [\hat{y}, \hat{L}_y] = [\hat{z}, \hat{L}_z] = 0$

$$[\hat{x}, \hat{L}_y] = [\hat{x}, \hat{z}\hat{p}_x] - [\hat{x}, \hat{x}\hat{p}_z] = [\hat{x}, \hat{z}]\hat{p}_x + \hat{z}[\hat{x}, \hat{p}_x] - [\hat{x}, \hat{x}]\hat{p}_z - \hat{x}[\hat{x}, \hat{p}_z] = i\hbar\hat{z}$$

$$[\hat{p}_x, \hat{L}_y] = [\hat{p}_x, \hat{z}\hat{p}_x] - [\hat{p}_x, \hat{x}\hat{p}_z] = [\hat{p}_x, \hat{z}]\hat{p}_x + \hat{z}[\hat{p}_x, \hat{p}_x] - [\hat{p}_x, \hat{x}]\hat{p}_z - \hat{x}[\hat{p}_x, \hat{p}_z] = i\hbar\hat{p}_z$$

to obtain $[\hat{x}, \hat{L}_y] = i\hbar\hat{z}, \quad [\hat{p}_x, \hat{L}_y] = i\hbar\hat{p}_z,$

and similarly $[\hat{x}, \hat{L}_z] = -i\hbar\hat{y}, \quad [\hat{p}_x, \hat{L}_z] = -i\hbar\hat{p}_y$

8. Angular Momentum

- Using cyclic symmetry $\hat{x} \to \hat{y};\quad \hat{y} \to \hat{z};\quad \hat{z} \to \hat{x}$ we get also:

$$\left[\hat{y},\hat{L}_x\right] = -i\hbar\hat{z},\quad \left[\hat{p}_y,\hat{L}_x\right] = -i\hbar\hat{p}_z,\qquad \left[\hat{z},\hat{L}_x\right] = i\hbar\hat{y},\quad \left[\hat{p}_z,\hat{L}_x\right] = i\hbar\hat{p}_y,$$
$$\left[\hat{y},\hat{L}_z\right] = i\hbar\hat{x},\quad \left[\hat{p}_y,\hat{L}_z\right] = i\hbar\hat{p}_x\qquad \left[\hat{z},\hat{L}_y\right] = -i\hbar\hat{x},\quad \left[\hat{p}_z,\hat{L}_y\right] = -i\hbar\hat{p}_x$$

  – A shorthand way of writing these relationships is:

$$\left[\hat{x}_i,\hat{L}_j\right] = i\hbar\varepsilon_{ijk}\hat{x}_k \qquad \left[\hat{p}_i,\hat{L}_j\right] = i\hbar\varepsilon_{ijk}\hat{p}_k \qquad \text{with}\quad \varepsilon_{ijk} = \begin{cases} 1 & ijk = 123, 231, 312 \\ -1 & ijk = 321, 213, 132 \\ 0 & \text{otherwise} \end{cases}$$

Levi-Civita antisymmetric tensor

- Commutation relations of the angular momentum:

$$\left[\hat{L}_x,\hat{L}_y\right] = \left[\hat{y}\hat{p}_z - \hat{z}\hat{p}_y,\hat{L}_y\right] = \hat{y}\left[\hat{p}_z,\hat{L}_y\right] + \left[\hat{y},\hat{L}_y\right]\hat{p}_z - \hat{z}\left[\hat{p}_y,\hat{L}_y\right] - \left[\hat{z},\hat{L}_y\right]\hat{p}_y = -i\hbar\hat{y}\hat{p}_x + i\hbar\hat{x}\hat{p}_y = i\hbar\hat{L}_z$$

- Based on symmetry $\hat{x} \to \hat{y};\quad \hat{y} \to \hat{z};\quad \hat{z} \to \hat{x}$ we have:

$$\left[\hat{L}_x,\hat{L}_y\right] = i\hbar\hat{L}_z;\quad \left[\hat{L}_y,\hat{L}_z\right] = i\hbar\hat{L}_x;\quad \left[\hat{L}_z,\hat{L}_x\right] = i\hbar\hat{L}_y$$

8. Angular Momentum

- A shorthand way of writing all three commutator relations is:

$$\underline{\hat{L}} \times \underline{\hat{L}} = i\hbar\underline{\hat{L}}$$

$$\begin{vmatrix} \underline{u}_x & \underline{u}_y & \underline{u}_z \\ \hat{L}_x & \hat{L}_y & \hat{L}_z \\ \hat{L}_x & \hat{L}_y & \hat{L}_z \end{vmatrix} = \underline{u}_x\left(\hat{L}_y\hat{L}_z - \hat{L}_z\hat{L}_y\right) + \underline{u}_y\left(\hat{L}_z\hat{L}_x - \hat{L}_x\hat{L}_z\right) + \underline{u}_z\left(\hat{L}_x\hat{L}_y - \hat{L}_y\hat{L}_x\right) = i\hbar\left(\underline{u}_x\hat{L}_x + \underline{u}_y\hat{L}_y + \underline{u}_z\hat{L}_z\right)$$

  – Because the three commutator relations are non-zero, the components of the angular momentum are not compatible, so we cannot have simultaneous eigenstates of L_x and L_y, of L_y and L_z or of L_x and L_z.

- The square of the angular momentum is: $\hat{L}^2 = \hat{L}_x^2 + \hat{L}_y^2 + \hat{L}_z^2$

$$\left[\hat{L}_z,\hat{L}^2\right] = \left[\hat{L}_z,\hat{L}_x^2\right] + \left[\hat{L}_z,\hat{L}_y^2\right] + \left[\hat{L}_z,\hat{L}_z^2\right] = \left[\hat{L}_z,\hat{L}_x\right]\hat{L}_x + \hat{L}_x\left[\hat{L}_z,\hat{L}_x\right] + \left[\hat{L}_z,\hat{L}_y\right]\hat{L}_y + \hat{L}_y\left[\hat{L}_z,\hat{L}_y\right] =$$
$$= i\hbar\hat{L}_y\hat{L}_x + i\hbar\hat{L}_x\hat{L}_y - i\hbar\hat{L}_x\hat{L}_y - i\hbar\hat{L}_y\hat{L}_x = 0$$

Similarly: $\left[\hat{L}_x,\hat{L}^2\right] = \left[\hat{L}_y,\hat{L}^2\right] = 0 \quad \Rightarrow \quad \left[\underline{\hat{L}},\hat{L}^2\right] = 0$

Therefore, it is possible to have simultaneous eigenstates of L^2 and L_z. These can define a **complete set of observables** for the angular momentum. Note that we could have also chosen L^2 *and* L_x or L^2 *and* L_y.

8. Angular Momentum

- It is convenient to work in polar coordinates:

$$x = r\sin\theta\cos\varphi \qquad y = r\sin\theta\sin\varphi \qquad z = r\cos\theta$$

$$\Rightarrow \quad \underline{\nabla} = \underline{u}_r \frac{\partial}{\partial r} + \underline{u}_\theta \frac{1}{r}\frac{\partial}{\partial \theta} + \underline{u}_\varphi \frac{1}{r\sin\theta}\frac{\partial}{\partial \varphi}$$

$$\underline{r} = \underline{u}_r r$$

– Therefore:

$$\underline{\hat{L}} = -i\hbar \underline{r} \times \underline{\nabla} = -i\hbar\left(\underline{u}_\varphi \frac{\partial}{\partial \theta} - \underline{u}_\theta \frac{1}{\sin\theta}\frac{\partial}{\partial \varphi}\right)$$

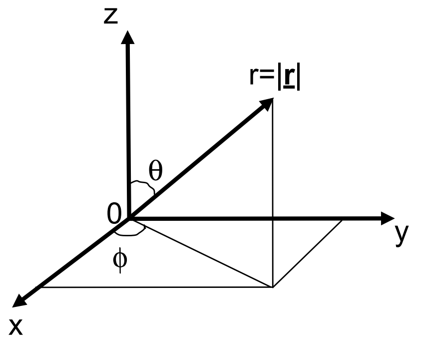
no radial dependence - L does not depend on $\underline{u}_r$

– The components of the operator will be:

$$\hat{L}_x = -i\hbar\left(-\sin\varphi \frac{\partial}{\partial \theta} - \cot\theta\cos\varphi \frac{\partial}{\partial \varphi}\right)$$

$$\hat{L}_y = -i\hbar\left(-\cos\varphi \frac{\partial}{\partial \theta} - \cot\theta\sin\varphi \frac{\partial}{\partial \varphi}\right)$$

$$\boxed{\hat{L}_z = -i\hbar \frac{\partial}{\partial \varphi}}$$



$$r \geq 0, \quad 0 \leq \theta \leq \pi, \quad 0 \leq \varphi \leq 2\pi$$

8. Angular Momentum

– The square of the angular momentum can be calculated with:

$$\hat{L}^2 = -\hbar^2 (\underline{r}\times\underline{\nabla})\cdot(\underline{r}\times\underline{\nabla}) = -\hbar^2 \underline{r}\cdot\underline{\nabla}\times(\underline{r}\times\underline{\nabla})$$

$$= -\hbar^2 \underline{r}\cdot\underline{\nabla}\times\left(\underline{u}_\varphi \frac{\partial}{\partial \theta} - \underline{u}_\theta \frac{1}{\sin\theta}\frac{\partial}{\partial \varphi}\right)$$

– Hence:

$$\boxed{\hat{L}^2 = -\hbar^2\left(\frac{1}{\sin\theta}\frac{\partial}{\partial \theta}\left(\sin\theta\frac{\partial}{\partial \theta}\right) + \frac{1}{\sin^2\theta}\frac{\partial^2}{\partial \varphi^2}\right)}$$

– We will choose L^2 and L_z as our compatible set of observables for angular momentum.

– We perform a separation of variables by introducing:

$$Y_{lm}(\theta,\varphi) = \Theta(\theta)\,\Phi(\varphi)$$

8. Angular Momentum

- Eigenfunctions and eigenvalues of $\hat{L}_z = -i\hbar \frac{\partial}{\partial \varphi}$:
  - Let us write the eigenvalues as $m\hbar$:

$$\hat{L}_z \Phi_m(\varphi) = m\hbar \Phi_m(\varphi) \quad \Rightarrow \quad -i \frac{\partial}{\partial \varphi} \Phi_m(\varphi) = m \Phi_m(\varphi)$$

  - Solution: $\Phi_m(\varphi) = \dfrac{1}{(2\pi)^{1/2}} e^{im\varphi}$
  - For the solution to be single-valued in $\varphi=0$ we must have:

$$e^{i2\pi m} = 1 \quad \Rightarrow \quad m = 0, \pm 1, \pm 2, \ldots$$

"magnetic quantum number"

i.e. the z-component of the orbital angular momentum is quantised.

  - Then the eigenvalues of L_z are: $0, \pm\hbar, \pm 2\hbar, \ldots$
  - Notice that, again, quantisation comes from imposing a boundary condition.

8. Angular Momentum

- Simultaneous eigenfunctions of L^2 and L_z:
  - Let us assume that the eigenvalues of L^2 are $l(l+1)\hbar^2$. Since $Y_{lm}(\theta,\phi)$ are common eigenfunctions of the two operators, then:

$$\hat{L}^2 Y_{lm}(\theta,\varphi) = l(l+1)\hbar^2 Y_{lm}(\theta,\varphi)$$
$$\hat{L}_z Y_{lm}(\theta,\varphi) = m\hbar Y_{lm}(\theta,\varphi)$$

we will see later on why

  - In polar coordinates:

$$-\left(\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right) + \frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\varphi^2}\right) Y_{lm}(\theta,\varphi) = l(l+1) Y_{lm}(\theta,\varphi)$$

$$\Rightarrow \left(\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right) + \left\{ l(l+1) - \frac{m^2}{\sin^2\theta} \right\}\right) \Theta_{lm}(\theta) = 0$$

  - Physical solutions must be in the range $-\pi/2 \le \theta \le \pi/2$. We can do a change of variable to $F_{lm}(w) = \Theta_{lm}(\theta) \quad \text{where} \quad w = \cos\theta \quad (-1 \le w \le 1)$

  and write: $$\left((1-w^2)\frac{d^2}{dw^2} - 2w\frac{d}{dw} + l(l+1) - \frac{m^2}{1-w^2} \right) F_{lm}(w) = 0$$

8. Angular Momentum

- For m=0:

$$\left((1-w^2)\frac{d^2}{dw^2} - 2w\frac{d}{dw} + l(l+1)\right)F_{l0}(w) = 0$$

This is Legendre's differential equation. Its solutions are the Legendre polynomials $P_l(w)$:

$$P_l(w) = \frac{1}{2^l l!}\frac{d^l}{dw^l}\left[(w^2-1)^l\right]$$

Recursively: $P_0(w) = 1, \quad P_1(w) = w$

$$(l+1)P_{l+1}(w) = (2l+1)wP_l(w) - lP_{l-1}(w)$$

- After normalisation we have our solution as a polynomial of order l: $F_{l0}(w) = \left(\frac{2l+1}{2}\right)^{1/2} P_l(w)$

8. Angular Momentum

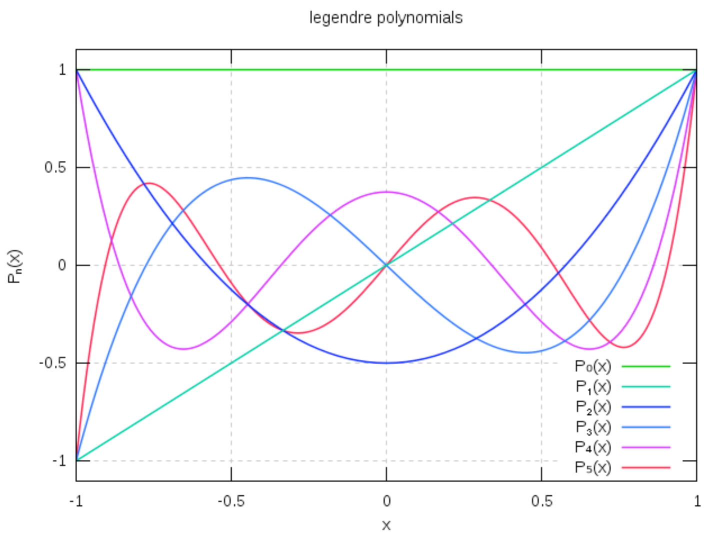
- The Legendre polynomials are orthogonal polynomials with alternating odd and even symmetry. Orthogonality:

$$\int_{-1}^{1} P_m(w)P_n(w)dw = \frac{2}{2n+1}\delta_{mn} \qquad \text{where} \qquad \delta_{mn} = \begin{cases} 1 & if \quad m=n \\ 0 & otherwise \end{cases}$$

Kronecker delta

- The first six Legendre polynomials:

$$P_0(w) = 1$$
$$P_1(w) = w$$
$$P_2(w) = \frac{1}{2}\left(3w^2 - 1\right)$$
$$P_3(w) = \frac{1}{2}\left(5w^3 - 3w\right)$$
$$P_4(w) = \frac{1}{8}\left(35w^4 - 30w^2 + 3\right)$$
$$P_5(w) = \frac{1}{8}\left(63w^5 - 70w^3 + 15w\right)$$



8. Angular Momentum

- Adrien-Marie Legendre (1752-1833)
  - French mathematician
  - Worked on number theory, statistics, algebra, analysis, celestial mechanics, elliptic integrals, Fermat's last theorem for n=5, …
  - Named after him: Legendre transformation, Legendre differential equation, Legendre polynomials, Legendre symbol, etc.
  - His work inspired or was the starting point for work done by Abel, Galois and Gauss
  - His name is one of the 72 names inscribed on the Eiffel Tower
  - Like Hermite, he could not have anticipated the use of his equations in Quantum Mechanics

Watercolor caricature of Legendre by artist Julien-Leopold Boilly (1820)