The Associated Legendre Functions are simple polynomials in both $\cos\theta$ and $\sin\theta$. They arise as the solutions of the θ-equation that is separated from equations like

$$-\Delta\phi = k^2\phi .$$

The θ-equation is

$$\frac{1}{\sin\theta}\frac{d}{d\theta}\left(\sin\theta\,\frac{dP_n^m(\cos\theta)}{d\theta}\right) + \left[n(n+1) - \frac{m^2}{\sin^2\theta}\right]P_n^m(\cos\theta) = 0$$

or with $x = \cos\theta$

$$\left[(1-x^2)\,P_n^{m\prime}(x)\right]' + \left[n(n+1) - \frac{m^2}{1-x^2}\right]P_n^m(x) = 0 \qquad (*)$$

which is self adjoint.

To get $P_n^m(x)$, we use Leibnitz's rule

$$\frac{d^n}{dx^n}AB = \sum_{s=0}^{n}\binom{n}{s}A^{(n-s)}B^{(s)}$$ to differentiate

Legendre's equation

$$\left[(1-x^2)P_n'\right]' + n(n+1)P_n = 0$$

m times, obtaining

$$(1-x^2)u'' - 2x(m+1)u' + (n-m)(n+m+1)u = 0$$

where $u = P_n^{(m)} = \dfrac{d^m}{dx^m}P_n(x)$.

We make this equation self adjoint by setting

$$v(x) = (1-x^2)^{\frac{m}{2}} u(x) = (1-x^2)^{\frac{m}{2}} \frac{d^m}{dx^m} P_n(x),$$

whence, after some work, we get

$$[(1-x^2)v']' + \left[n(n+1) - \frac{m^2}{1-x^2}\right]v = 0$$

which is Eq. (*). So apart from a scale factor,

$$P_n^m(x) = (1-x^2)^{\frac{m}{2}} \frac{d^m}{dx^m} P_n(x).$$

The scale factor is unity.

Because R's formula for P_n is

$$P_n(x) = \frac{1}{2^n n!} \left(\frac{d}{dx}\right)^n (x^2-1)^n$$

$$P_n^m(x) = \frac{(1-x^2)^{\frac{m}{2}}}{2^n n!} \left(\frac{d}{dx}\right)^{n+m} (x^2-1)^n$$

makes perfect sense as long as $n+m \geq 0$.
In fact,

$$P_n^{-m}(x) = (-1)^m \frac{(n-m)!}{(n+m)!} P_n^m(x).$$

Indeed, since m occurs only as m^2, P_n^{-m} would have to be proportional to P_n^m.

$$P_n^0 = P_n$$

Recurrence relations and a generating function are given by Eqs. (12.83-89) of the text.

Parity

$$P_n^m(-x) = (-1)^{n+m} P_n^m(x).$$

$P_n^m(\pm 1) = 0$ for $m \neq 0$ due to the factor $(1-x^2)^{m/2}$.

Orthogonality

$$\int_{-1}^{1} P_p^m(x)\, P_q^m(x)\, dx = \frac{2}{2q+1} \frac{(q+m)!}{(q-m)!} \delta_{p,q}$$

$$\| \qquad\qquad //$$

$$\int_0^{\pi} P_p^m(\cos\theta)\, P_q^m(\cos\theta) \sin\theta\, d\theta$$

Also

$$\int_{-1}^{1} P_n^m(x)\, P_n^k(x) \frac{dx}{(1-x^2)} = \frac{(n+m)!}{m(n-m)!} \delta_{m,k}$$

which is rarely useful.

Spherical Harmonics

$$-\Delta\psi = k^2 f(n)\,\psi \quad \text{is separable.}$$

The angular part is

$$\frac{\Phi}{\sin\theta}\frac{d}{d\theta}\left(\sin\theta\frac{d\Theta}{d\theta}\right) + \frac{\Theta}{\sin^2\theta}\frac{d^2\Phi}{d\phi^2} + (n+1)n\,\Theta\Phi = 0$$

We take

$$\Phi_m(\phi) = \frac{e^{im\phi}}{\sqrt{2\pi}}$$

and

$$\Theta_n^m(\theta) = (-1)^m\sqrt{\frac{2n+1}{2}\frac{(n-m)!}{(n+m)!}}\;P_n^m(\cos\theta)$$

and set

$$Y_n^m(\theta,\phi) = \Theta_n^m(\theta)\,\Phi_m(\phi)$$

$$= (-1)^m\sqrt{\frac{2n+1}{4\pi}\frac{(n-m)!}{(n+m)!}}\;P_n^m(\cos\theta)\,e^{im\phi}$$

so that

$$\int_0^{2\pi}d\phi\int_0^{\pi}d\theta\,\sin\theta\;Y_n^{m*}(\theta,\phi)\;Y_{n'}^{m'}(\theta,\phi) = \delta_{nn'}\delta_{mm'}.$$

The Y_n^m's are polynomials in $\sin\theta$, and $\cos\theta$ multiplied by $e^{im\phi}$.

The Y_ℓ^m's are complete for functions defined on the unit sphere. An example is

$$P_\ell(\hat{r}\cdot\hat{r}') = \frac{4\pi}{2\ell+1}\sum_{m=-\ell}^{\ell} Y_\ell^m(\theta,\phi)\,Y_\ell^{m*}(\theta',\phi')$$

More generally, if

$$f(\theta,\phi) = \sum_{mn} a_{mn} Y_n^m(\theta,\phi)$$

or

$$f(\Omega) = \sum_{mn} a_{mn} Y_n^m(\Omega),$$ then

$$\int d\Omega\, f(\Omega)\, Y_n^{m*}(\Omega) = \int_0^{2\pi} d\phi \int_0^{\pi} d\theta \sin\theta\, f(\theta,\phi)\, Y_n^{m*}(\theta,\phi)$$

$$= a_{mn}.$$ So

$$f(\Omega) = \sum_{mn} Y_n^m(\Omega)\int d\Omega'\, f(\Omega')\, Y_n^{m*}(\Omega')$$

$$= \int d\Omega'\, f(\Omega') \sum_{mn} Y_n^m(\Omega)\, Y_n^{m*}(\Omega')$$ so

$$\delta(\Omega-\Omega') = \sum_{n=0}^{\infty}\sum_{m=-n}^{n} Y_n^m(\Omega)\, Y_n^{m*}(\Omega').$$

Another example: for $R > r$,

$$\frac{1}{|\vec{r} - \vec{R}|} = \frac{1}{R} \sum_{l=0}^{\infty} \sum_{m=-l}^{l} \frac{4\pi}{2m+1} \left(\frac{r}{R}\right)^l Y_l^{m*}(\Omega_r) Y_l^m(\Omega_R)$$

follows from

$$\frac{1}{|r - R|} = \frac{1}{R} \sum_{l=0}^{\infty} \left(\frac{r}{R}\right)^l P_l(\hat{r} \cdot \hat{R})$$

and

$$P_m(\hat{r} \cdot \hat{R}) = \frac{4\pi}{2l+1} \sum_{m=-l}^{l} Y_l^m(\hat{r}) Y_l^{m*}(\hat{R})$$

$$= \frac{4\pi}{2l+1} \sum_{m=-l}^{l} Y_l^m(\hat{R}) Y_l^{m*}(\hat{r}).$$

$$\vec{L} = \frac{\hbar}{i} \vec{r} \times \vec{\nabla}$$

$$[L_i, L_j] = i\hbar \, \epsilon_{ijk} L_k$$

$$\vec{L} \cdot \vec{L} \, Y_l^m(\hat{r}) = L^2 Y_l^m(\hat{r})$$

$$= -\hbar^2 \left[\frac{1}{\sin\theta} \frac{\partial}{\partial\theta}\left(\sin\theta \frac{\partial}{\partial\theta}\right) + \frac{1}{\sin^2\theta} \frac{\partial^2}{\partial\varphi^2} \right] Y_l^m(\hat{r})$$

$$= l(l+1)\hbar^2 \, Y_l^m(\hat{r}).$$

The Calculus of Variations

As we saw when we discussed path integrals, the amplitude

$$\langle \phi | \psi, T \rangle = \langle \phi | e^{-iTH/\hbar} | \psi \rangle = \langle \phi | e^{-iT\left(\frac{p^2}{2m} + V(x)\right)/\hbar} | \psi \rangle$$

$$= \int Dx(t) \, e^{iS[x]/\hbar} \langle \phi | x(T) \rangle \langle x(0) | \psi \rangle$$

where $S[x]$ is the classical action

$$S[x(t)] = \int_0^T dt \; L(x, \dot{x}) = \int_0^T dt \left[\frac{m}{2} \dot{x}^2(t) - V(x(t)) \right].$$

Two paths that differ by $\delta x(t)$ may wash each other out unless the action S is stationary,

$0 = \delta S$, which means that $\delta S \propto \delta x^2$.
This is the principle of least action.

In fact, much of classical physics follows from a choice of S and the rule $0 = \delta S$.

Example: (Note $\delta \dot{x} = \dot{x} + \dot{\delta x} - \dot{x} = d\,\delta x/dt$.)

$$\delta S = \int_0^T dt \quad m \dot{x} \, \delta \dot{x} - V' \delta x \quad + \quad \mathcal{O}(\delta x^2)$$

$$= \int_0^T dt \; - \delta x \left(m \ddot{x} + V' \right) \quad + \left[m \dot{x} \, \delta x \right]_0^T ,$$

since we dropped δx^2.

If the two paths $x(t)$ and $x(t) + \delta x(t)$ both go from $x(0)$ to $x(T)$, then

$$\delta x(0) = \delta x(T) = 0$$

and the boundary terms vanish. Then

$$\delta S = - \int_0^T dt \, (m\ddot{x} + V')\delta x$$

So if $\delta S \propto \delta x^2$, ~~and~~ not $\delta \propto \delta x$, then

$$0 = \delta S = - \int_0^T dt \, (m\ddot{x} + V')\delta x$$

and since δx is arbitrary (but small), we get

$$m\ddot{x} + V' = 0 \quad \text{or} \quad m\ddot{x} = -V' \quad \text{or}$$

$$m\ddot{x} = F = ma = \frac{\partial V(x)}{\partial x}.$$

In books on classical mechanics, one often uses generalized coordinates $q_i(t)$ so that

$$S = \int_0^T dt \, L(q, \dot{q}, t),$$

in which q and $\dot{q}$ stand for $q_1 \cdots q_N$, etc.

Now the action S will be stationary if

$$0 = \delta S = \int_0^T dt \left(\frac{\partial L}{\partial q_i} \delta q_i + \frac{\partial L}{\partial \dot{q}_i} \delta \dot{q}_i \right).$$

Now

$$\delta \dot{q}_i = \dot{q}_i + \delta \dot{q}_i - \dot{q}_i = \frac{d}{dt} \delta q_i, \text{ so}$$

again integrating by parts, we have

$$\delta S = \int_0^T dt \; \delta q_i \left(\frac{\partial L}{\partial q_i} - \frac{d}{dt} \frac{\partial L}{\partial \dot{q}_i} \right) + \left[\frac{\partial L}{\partial \dot{q}_i} \delta q_i \right]_0^T .$$

If all the paths go from $q_i(0)$ to $q_i(T)$, then

$\delta q_i(0) = \delta q_i(T) = 0$ and we have

$$0 = \delta S \quad \text{if} \qquad \frac{\partial L}{\partial q_i} - \frac{d}{dt} \frac{\partial L}{\partial \dot{q}_i} = 0 .$$

The canonical momentum p_i is

$$p_i = \frac{\partial L}{\partial \dot{q}_i} \qquad \text{and so}$$

Lagrange's equations imply $\quad \dot{p}_i = \dfrac{\partial L}{\partial q_i}$.

Usually the Lagrangian $L(q,\dot{q})$ does not involve t explicitly. In this case, one may define a hamiltonian H that is conserved:

$$H = \sum_{i=1}^{N} p_i \dot{q}_i - L$$

To see that $\dot{H}$ vanishes, just take its time derivative

$$\dot{H} = \sum_{i=1}^{N} \left(\dot{p}_i \dot{q}_i + p_i \ddot{q}_i - \frac{\partial L}{\partial q_i} \dot{q}_i - \frac{\partial L}{\partial \dot{q}_i} \ddot{q}_i \right)$$

But $p_i = \dfrac{\partial L}{\partial \dot{q}_i}$ and $\dot{p}_i = \dfrac{\partial L}{\partial q_i}$, so $\dot{H} = 0$.

Now suppose $\mathcal{L}(\phi, \phi_{,j})$ is a Lagrange density that depends on the fields $\phi_1, \phi_2 \cdots \phi_N$ and their derivatives

$$\phi_{i,j} = \frac{\partial \phi_i}{\partial x_j} .$$

Assume that $\delta\phi_i = 0$ when any argument $x_k \to \pm\infty$, so we can drop all surface terms. Then

$$L = \int d^3x \, \mathcal{L} \quad \text{and} \quad S = \int dt \, L = \int d^4x \, \mathcal{L} .$$

The requirement that δS be quadratic or higher in $\delta\phi$ gives

$$0 = \delta S = \int d^4x \, \frac{\partial \mathcal{L}}{\partial \phi_i} \delta\phi_i + \frac{\partial \mathcal{L}}{\partial \phi_{i,j}} \delta\phi_{i,j}$$

Now $\delta\phi_{i,j} = (\phi_i + \delta\phi_i)_{,j} - \phi_{i,j} = (\delta\phi_i)_{,j}$

where $G_{,j} = \dfrac{\partial G}{\partial x_j}$, as before. So

$$0 = \delta S = \int d^4x \;\; \delta\phi_i \left(\frac{\partial \mathcal{L}}{\partial \phi_i} - \left(\frac{\partial \mathcal{L}}{\partial \phi_{i,j}} \right)_{,j} \right) + \underset{\displaystyle 0}{\underset{\|}{S.T.}}$$

whence the field equations

$$0 = \frac{\partial \mathcal{L}}{\partial \phi_i} - \frac{\partial}{\partial x_j}\left(\frac{\partial \mathcal{L}}{\partial \phi_{i,j}} \right).$$

In this way, one does field theory.

Lagrange Multipliers

Suppose one wants to find x and y that maximize $f(x,y)$ subject to the constraint $g(x,y) = c$, a constant. Set

$$H(x,y,\lambda) = f(x,y) + \lambda\,(g(x,y) - c)$$

and find the $x, y,$ & λ that maximize H. Then

$$\left.\begin{aligned} 0 = \frac{\partial H}{\partial x} = H_x &= f_x + \lambda g_x = 0 \\ 0 = H_y &= f_y + \lambda g_y = 0 \\ 0 = H_\lambda &= g - c = 0. \end{aligned}\right\} \text{Solve these three eqs. for } x, y, \text{ and } \lambda.$$

Why does this work? Well, one could solve for the curve $y(x)$ that keeps

$$g(x, y(x)) = c.$$

then one can maximize $f(x, y(x))$ by setting its derivative equal to zero:

$0 = f_x + y' f_y$. To find y', one sets

$0 = g_x + y' g_y$, which gives $y' = -\frac{1}{g_y} g_x$.

So

$$0 = f_x + y' f_y = f_x - \frac{1}{g_y} g_x f_y \quad \text{or}$$

$$0 = f_x - \frac{f_y}{g_y} g_x \qquad \text{ie} \quad \lambda = -\frac{f_y}{g_y}$$

and

$$0 = f_y + \frac{1}{y'} f_x$$

$$0 = f_y - \frac{g_y}{g_x} f_x = f_y - \frac{f_x}{g_x} g_y \quad \text{ie } \lambda = -\frac{f_x}{g_x}.$$

So

$$0 = f_x - \frac{f_y}{g_y} g_x$$

$$0 = f_y - \frac{f_x}{g_x} g_y$$

and the two equations for λ are the same because

$$0 = f_x - \frac{g_x}{g_y} f_y \quad \text{which means} \quad \frac{f_x}{g_x} = \frac{f_y}{g_y} = -\lambda.$$

Suppose $\rho = \sum p_n |n\rangle\langle n|$ is a density operator. Then $\langle F \rangle = \mathrm{tr}(\rho F)$

and $1 = \langle 1 \rangle = \mathrm{tr}\,\rho$. And $\langle H \rangle = \mathrm{tr}\,\rho H$.

Now $S = -k\,\mathrm{tr}(\rho \log \rho)$. So let's maximize S subject to the conditions $1 = \mathrm{tr}\,\rho$ and $E = \langle H \rangle$.

So we maximize

$$Z(\rho, \lambda, \mu) = S + \lambda(E - \langle H \rangle) + \mu(1 - \langle 1 \rangle)$$

$$= -k\,\mathrm{tr}(\rho \log \rho) + \lambda(E - \mathrm{tr}\,H\rho) + \mu(1 - \mathrm{tr}\,\rho)$$

We suppose $\langle n | n' \rangle = \delta_{nn'}$

$$H|n\rangle = E_n |n\rangle. \quad \text{So}$$

$$Z(\rho, \lambda, \mu) = -k \sum \rho_n \log \rho_n + \lambda\left(E - \sum \rho_n E_n\right) + \mu\left(1 - \sum \rho_n\right)$$

$$0 = \frac{\partial Z}{\partial \rho_n} = -k \log \rho_n - \lambda E_n - \mu, \quad \text{so}$$

$$\log \rho_n = (-\lambda E_n - \mu)/k$$

$$\rho_n = e^{(-\lambda E_n - \mu)/k}$$

Choose μ, by setting $\rho_n = \dfrac{e^{-\frac{\lambda E_n}{k}}}{\sum_n e^{-\lambda E_n / k}}$.

Choose $\lambda = \frac{1}{T}$

by the rule $\sum \rho_n E_n = E$.

Then

$$\rho_n = \frac{e^{-\frac{E_n}{kT}}}{\sum_n e^{-E_n/kT}}$$

is the quantum density operator that maximizes entropy for a fixed mean value $\bar{E}$ of the energy while conserving probability
$\mathrm{tr}\,\rho = 1$.