PHYSICS 580: Quantum Mechanics I.

Notes on Sturm-Liouville Theory and Orthogonal Polynomials

1 Classification of Sturm-Liouville 2nd Order Differential Equations

Many special functions that appear in physics are solutions to second order ordinary differential equations of the form

$$Lf = \lambda f$$

where

$$L = a(x)\frac{d^2}{dx^2} + b(x)\frac{d}{dx} + c(x), \tag{1}$$

for some *real* functions $a(x), b(x), c(x)$ and a constant λ. We will call the constant λ an eigenvalue of the operator L.

In QM, the eigenvalues of observables are real numbers, so we need to impose that L is Hermitian with respect to an inner product $\langle \, , \, \rangle$ defined on the Hilbert space of functions on which L acts. Let us define the inner product as a weighted integral

$$\langle f, g\rangle = \int_{-\infty}^{\infty} f^*(x)g(x)w(x)dx$$

where, if possible, we need to choose the weight $w(x)$ appropriately for given $a(x), b(x)$, and $c(x)$, so that L becomes Hermitian. The Hermitian condition with respect to this inner product is $\langle Lf, g\rangle = \langle f, Lg\rangle$, i.e. we want to choose $w(x)$ such that

$$\langle Lf, g\rangle - \langle f, Lg\rangle = 0. \tag{2}$$

Integrating by parts the second derivative terms, we get

$$\begin{aligned}\langle Lf, g\rangle - \langle f, Lg\rangle &= \int_{-\infty}^{\infty} \left[(af^{*\prime\prime} + bf^{*\prime})g - f^*(ag'' + bg')\right] w dx \\ &= aw(f^{*\prime}g - f^*g')|_{-\infty}^{\infty} + \int_{-\infty}^{\infty} (bw - (aw)')(f^{*\prime}g - f^*g')dx,\end{aligned}$$

which vanishes for all $f(x)$ and $g(x)$ if

$$\boxed{aw(f^{*\prime}g - f^*g')|_{-\infty}^{\infty} = 0} \tag{3}$$

$$\boxed{(aw)' = bw} \tag{4}$$

Rewriting (4) as

$$(aw)' = \frac{b}{a}(aw)$$

and integrating gives

$$w \propto \frac{e^{\int \frac{b}{a} dx}}{a}. \tag{5}$$

Hence, imposing that L is Hermitian completely specifies w in terms of $a(x)$ and $b(x)$ in the region where $(aw)'$ is continuous. We then need to choose $a(x)$ and $b(x)$ so that (3) is satisfied.

We are particularly interested in finding conditions on $a(x), b(x)$, and $c(x)$, so that (1) has polynomial solutions of the form

$$Q_n(x) = \alpha_n^{(n)} x^n + \alpha_{n-1}^{(n)} x^{n-1} + \cdots + \alpha_0^{(n)}, \text{ where } \alpha_k^{(n)} \in \mathbb{R}, \alpha_n^{(n)} \neq 0,$$

that satisfy $LQ_n(x) = \lambda_n Q_n(x)$, for $n = 0, 1, \ldots$ Let us first impose $LQ_0(x) = \lambda_0 Q_0(x)$. Since $Q_0(x) = \alpha_0^{(0)}$, we have

$$c(x)\alpha_0^{(0)} = \lambda \alpha_0^{(0)} \Rightarrow c(x) = \lambda_0.$$

So, $c(x)$ has to be a constant; let's call this constant c. Similarly, let us impose $LQ_1(x) = \lambda_1 Q_1(x)$:

$$b(x)\alpha_1^{(1)} + c(\alpha_1^{(1)} x + \alpha_0^{(1)}) = \lambda_1(\alpha_1^{(1)} x + \alpha_0^{(1)}) \Rightarrow b(x) = b_1 x + b_0.$$

Hence, $b(x)$ can be at most degree 1. Finally, imposing the condition $LQ_2(x) = \lambda_2 Q_2(x)$ implies that $a(x) = a_2 x^2 + a_1 x + a_0$. Hence, if L has polynomial solutions Q_n for all positive degrees n, then its most general form is

$$L = (a_2 x^2 + a_1 x + a_0)\frac{d^2}{dx^2} + (b_1 x + b_0)\frac{d}{dx} + c,$$

where a_i, b_i, c are real constants. Because c is just a multiplicative constant, we can absorb the term $cQ_n(x)$ into $\lambda_n Q_n(x)$, and just search for solutions to

$$\boxed{LQ_n(x) = \lambda_n Q_n(x), \text{ where } L = (a_2 x^2 + a_1 x + a_0)\frac{d^2}{dx^2} + (b_1 x + b_0)\frac{d}{dx}} \tag{6}$$

Collecting the x^n terms in (6) gives

$$a_2 n(n-1)\alpha_n^{(n)} + b_1 n \alpha_n^{(n)} = \lambda_n \alpha_n^{(n)} \Rightarrow \boxed{\lambda_n = n((n-1)a_2 + b_1)}.$$

We now need to choose a_0, a_1, a_2, b_0, b_1 in (6) so that (3) is satisfied. Up to scaling and shifting x and multiplying L by a constant, the possible values of a_0, a_1, a_2, b_0, b_1 are completely classified and they comprise the so-called Sturm-Liouville System:

Name	$a(x)$	$b(x)$	λ_n	$w(x)$	Support(w) $[\alpha, \beta]$
Jacobi $P_n^{\alpha,\beta}(x),\ \alpha, \beta > -1$	$1 - x^2$	$-(\alpha + \beta + 2)x + (\beta - \alpha)$	$-n((n-1) + (\alpha + \beta + 2)$	$(1-x)^\alpha(1+x)^\beta$	$[-1, 1]$
Chebyshev $T_n(x)$	$1 - x^2$	$-x$	$-n^2$	$(1-x^2)^{-1/2}$	$[-1, 1]$
Legendre $P_n(x) = P_n^{(0,0)}(x)$	$1 - x^2$	$-2x$	$-n(n+1)$	1	$[-1, 1]$
Laguerre $L_n^s(x),\ s > -1$	x	$s + 1 - x$	$-n$	$x^s e^{-x}$	$[0, \infty]$
Hermite $H_n(x)$	1	$-2x$	$-2n$	e^{-x^2}	$[-\infty, \infty]$

where w is 0 outside the indicated interval. Note that even if $w(x)$ may be discontinuous at α and β, the product aw is continuous and equal to 0 at these points, allowing us to solve for (4) by patching together the expression for aw obtained from (5) and $aw \equiv 0$ at the boundaries.

2 Polynomial Solutions

For each choice of a, b, and w, degree-n polynomial solutions to (6) are given by the Rodrigues formula:

Definition 2.1 (Rodrigues Formula)**.**

$$\boxed{Q_n(x) = K_n \frac{1}{w} \frac{d^n}{dx^n} \left[a(x)^n w(x)\right]} \tag{1}$$

where K_n is typically chosen so that

$$\int_{-\infty}^{\infty} Q_n(x) Q_n(x)\, w(x)\, dx = \int_{\alpha}^{\beta} Q_n(x) Q_n(x)\, w(x)\, dx = 1.$$

For Hermite polynomials, K_n is chosen to be $(-1)^n$ and the polynomials do not have a unit norm with respect to w. Note that we could change the limits of integration to $[\alpha, \beta]$ since $w(x)$ vanishes outside this interval.

To show that $Q_n(x)$ is indeed a degree-n polynomial, let us first prove the following:

Proposition 2.1. *Let $g_k(x)$ be any polynomial of degree k. Then,*

$$\frac{d}{dx}(a^n w g_k) = a^{n-1} w h_{k+1}$$

where $h_{k+1}(x)$ is some polynomial of degree $k+1$. Moreover, for $\ell \neq n$,

$$\frac{d^\ell}{dx^\ell}(a^n w g_k) = a^{n-\ell} w h_{k+\ell}$$

where $h_{k+\ell}(x)$ is some polynomial of degree $k+\ell$.

Proof. Writing $a^n w g_k = a^{n-1}(aw)g_k$ and using the product rule, we have

$$\frac{d}{dx}(a^n w g_k) = (n-1)a^{n-2}a'(aw)g_k + a^{n-1}(bw)g_k + a^{n-1}(aw)g_k'$$

where we used the condition (4), i.e. $\frac{d}{dx}(aw) = bw$. Factoring out $a^{n-1}w$, we get

$$\frac{d}{dx}(a^n w g_k) = a^{n-1} w \left[(n-1)a' g_k + b g_k + a g_k'\right].$$

Since $a(x)$ is quadratic and $b(x)$ is linear in x, we see that the quantity in the bracket is a polynomial of degree $k+1$. Repeating this procedure proves the second equation. □

Applying this Proposition to the case where $\ell = n$ and $g_k = 1$ yields

$$\frac{d^n}{dx^n}(a^n w) = w h_n$$

and thus proves

Proposition 2.2. *$Q_n(x)$ given by the Rodrigues Formula (1) is a degree n-polynomial.*

Proposition 2.1 also allows us to prove the following important orthogonoality relation:

Proposition 2.3. *For $m \neq n$, $Q_m(x)$ and $Q_n(x)$ defined by the Rodrigues Formula (1) are orthogonal with respect to the inner product defined by w, i.e.*

$$\int_{-\infty}^{\infty} Q_m(x) Q_n(x)\, w(x)\, dx = 0. \tag{2}$$

Proof. Without loss of generality, let us assume that $n > m$. Then,

$$\begin{aligned}
\int_{-\infty}^{\infty} Q_m(x) Q_n(x)\, w(x)\, dx &= \int_{\alpha}^{\beta} Q_m(x) K_n \frac{1}{w} \frac{d^n}{dx^n}\left[a(x)^n w(x)\right] w(x)\, dx \\
&= K_n \left(\sum_{k=0}^{n-1} (-1)^k \frac{d^k Q_m}{dx^k} \frac{d^{n-k-1}(a^n w)}{dx^{n-k-1}} \right) \Bigg|_{\alpha}^{\beta} \\
&\quad + (-1)^n K_n \int_{\alpha}^{\beta} \frac{d^n Q_m(x)}{dx^n} a^n w\, dx
\end{aligned}$$

Since the n-fold derivative of a degree-m polynomial is 0 for $n > m$, the last integral is 0. Using Proposition 2.1, the remaining sum can be expressed as

$$\int_{-\infty}^{\infty} Q_m(x) Q_n(x)\, w(x)\, dx = K_n \left(\sum_{k=0}^{n-1} (-1)^k \frac{d^k Q_m}{dx^k} \left(a^{k+1} w h_{n-k-1}\right) \right) \Bigg|_{\alpha}^{\beta}$$

But, since $aw = 0$ at the boundary points α and β, each sum is equal to 0. □

Checking that (1) indeed gives solutions to (6) by brute force computation is cumbersome. This fact, however, follows from the fact that the orthogonality condition (2) uniquely determines the polynomials $Q_n(x)$ up to multiplicative constants and that the eigen-polynomials of the Hermitian operator L have distinct eigenvalues and are thus also orthogonal with respect to $w(x)$. Thus, $Q_n(x)$ must be eigen-polynomials of L.

The utility of orthonomal polynomial solutions to a Sturm-Liouville differential equation stems from the fact that these polynomials are complete:

Theorem 2.1 (Completeness Theorem)**.** *The orthonomal set of polynomial solutions* $\{Q_n(x)\}_{n=0}^{\infty}$ *to a Sturm-Liouville system (6) is complete in the Hilbert space of square integrable functions defined on* $[\alpha, \beta]$*.*

In electrostatics, this theorem allows us to expand the angular part of electric potential in terms of Legendre polynomials. In QM, it gives an orthonormal basis of Hilbert space for SHO.

3 Example

Definition 3.1 (Legendre Polynomials ($a = 1 - x^2$, $b = -2x$, $w = 1$))**.** *The polynomial solutions to*

$$(1 - x^2)\frac{d^2 P_n}{dx^2} - 2x\frac{dP_n}{dx} + n(n+1)P_n = 0$$

satisfying

$$\int_{-1}^{1} P_n(x)P_m(x)dx = \delta_{m,n}$$

are given by

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

Definition 3.2 (Hermite Polynomials ($a = 1$, $b = -2x$, $w = e^{-x^2}$))**.** *The polynomial solutions to*

$$\frac{d^2 H_n}{dx^2} - 2x\frac{dH_n}{dx} + 2nH_n = 0$$

satisfying

$$\int_{-\infty}^{\infty} H_n(x)H_m(x)e^{-x^2}dx = \sqrt{\pi}\, 2^n n!\delta_{m,n}$$

are given by

$$H_n(x) = (-1)^n e^{x^2}\frac{d^n}{dx^n}e^{-x^2}.$$