DEPARTMENT OF PHYSICS
INDIAN INSTITUTE OF TECHNOLOGY, MADRAS

PH5100 Quantum Mechanics I **Problem Set 7** **11.9.2019**

Orthogonal Polynomials

We will encounter several second order differential equations in solving for the eigenfunctions of the Hamiltonian for several systems. Typically, after taking into account the asymptotic behaviour of the eigenfunction, we then look for *polynomial solutions* to a second-order equation. All the examples that we considered turn out to be differential equations of the **hypergeometric type**. A differential equation of the hypergeometric type is a second order ordinary differential equation of the form

$$\sigma(x)\,\frac{d^2\phi}{dx^2} + \tau(x)\,\frac{d\phi}{dx} + \lambda\,\phi = 0$$

where $\sigma(x)$ is a polynomial that is at most a quadratic in x, $\tau(x)$ is a polynomial that is at most a linear function of x, and λ is a constant. There is a very elaborate theory of hypergeometric equations and their solutions. Further let $\phi(x)$ be defined in the domain $[a, b]$ with norm

$$||\phi(x)||^2 = \int_a^b dx\ \rho(x)\ |\phi(x)|^2\ .$$

Note that the integration measure may **not** in general be the Lebesgue measure (unless the **weight function** $\rho(x)$ is unity).

The hypergometric equation has **polynomial solutions** $\phi_n(x)$ when λ takes on the special values

$$\lambda = \lambda_n = -n\,\tau\,' - \frac{1}{2}n(n-1)\,\sigma\,''\ ,$$

where a prime denotes the derivative with respect to x and n the degree of the polynomial. Such solutions are called **polynomials of the hypergeometric type**. Further, let the following additional condition imposed on the weight function $\rho(x):$ we require that

$$[\sigma(x)\,\rho(x)\,x^n]_{x=a} = 0\,,\quad [\sigma(x)\,\rho(x)\,x^n]_{x=b} = 0\,,\quad n = 0, 1, \ldots ..$$

There are basically three distinct families of such polynomials, essentially corresponding to the three distinct kinds of intervals: finite, semi-infinite, and infinite. After suitable changes of variables, they can be brought to the so-called canonical forms, given below. In each case we have a formula for the polynomial concerned, called the **Rodrigues formula**, which expresses the polynomial concerned as the nth derivative of a specific function of x, thus:

$$\phi_n(x) = \frac{(\mathrm{const.})_\mathrm{n}}{\rho(x)} \frac{d^n}{dx^n} [\sigma^n(x)\, \rho(x)] \quad (\textbf{Rodrigues formula}),$$

where $(\mathrm{const.})_n$ stands for an n-dependent constant. In practice, the Rodrigues formula provides a more convenient way of obtaining the polynomials.

(i) **Generalized Laguerre polynomials** $L_n^\alpha(x)$, where the constant $\alpha > -1$. In this case

$$(a,b) = (0,\infty),\ \sigma(x) = x,\ \rho(x) = x^\alpha\, e^{-x}.$$

The Rodrigues formula for generalized Laguerre polynomials is

$$L_n^\alpha(x) = \frac{1}{n!}\, x^{-\alpha}\, e^x\, \frac{d^n}{dx^n}\, (x^{n+\alpha}\, e^{-x}).$$

The generalized Laguerre polynomial satisfies the differential equation

$$x\, \frac{d^2y}{dx^2} + (\alpha - x + 1)\, \frac{dy}{dx} + n\, y = 0.$$

When the parameter $\alpha = 0$ the generalized Laguerre polynomial $L_n^\alpha(x)$ reduces to the (ordinary) **Laguerre polynomial**, denoted by $L_n(x)$: that is, $L_n^0(x) = L_n(x)$.

(ii) **Hermite polynomials** $H_n(x)$. In this case

$$(a,b) = (-\infty,\infty),\ \sigma(x) = 1,\ \rho(x) = e^{-x^2}.$$

The Rodrigues formula for Hermite polynomials is

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

$H_n(x)$ satisfies the differential equation

$$\frac{d^2y}{dx^2} - 2x\, \frac{dy}{dx} + 2n\, y = 0.$$

(iii) **Jacobi polynomials** $P_n^{(\alpha,\beta)}(x)$, where the constants $\alpha,\, \beta > -1$. In this case

$$(a,b) = (-1,1),\ \sigma(x) = 1 - x^2,\ \rho(x) = (1-x)^\alpha\, (1+x)^\beta.$$

The Rodrigues formula for Jacobi polynomials is

$$P_n^{(\alpha,\beta)}(x) = \frac{(-1)^n}{2^n\, n!}\,(1-x)^{-\alpha}(1+x)^{-\beta}\,\frac{d^n}{dx^n}\left[(1-x)^{n+\alpha}(1+x)^{n+\beta}\right].$$

$P_n^{(\alpha,\beta)}(x)$ satisfies the differential equation

$$(1-x^2)\,\frac{d^2y}{dx^2} + [\beta-\alpha-(\alpha+\beta+2)\,x]\,\frac{dy}{dx} + n(n+\alpha+\beta+1)\,y = 0\,.$$

when $\lambda = \frac{1}{2}$, i.e., when $\alpha = \beta = 0$, the Jacobi polynomial reduces to the very familiar **Legendre polynomial**, $P_n(x)$. The precise relationship is simply

$$P_n(x) = P_n^{(0,0)}(x)\,.$$

The associated Legendre polynomials are obtained from the Legendre polynomial as follows (for $0 \le m \le \ell$)

$$P_\ell^m(x) = (-1)^m (1-x^2)^{m/2}\left(\frac{d}{dx}\right)^m P_\ell(x)\ ,$$

$$P_\ell^{-m}(x) = (-1)^m \frac{(\ell-m)!}{(\ell+m)!}\,P_\ell^m(x)\ .$$

For fixed m, $P_\ell^m(x)$ form an orthogonal basis for functions on the interval $[-1,1]$ – this generalizes the earlier result for $m = 0$.

In the problems that follow, all symbols have their usual meaning as defined in the foregoing. Thus (a,b) is a general interval, $\{\phi_n(x)\}$ a family of orthogonal polynomials defined in this interval with weight function $\rho(x)$, and so on.

1. Show that, for any given n,

$$\int_a^b \phi_n(x)\, x^m\, \rho(x)\, dx = 0 \quad \text{for all } m < n\,.$$

   Hence each $\phi_n(x)$ is orthogonal to every polynomial of degree less than n.

2. Let $f(x) = \sum_n f_n \phi_n(x)$ be a square integrable function in (a,b). Show that

$$\sum_{n=0}^{\infty} A_n\, f_n^2 = \int_a^b f^2(x)\,\rho(x) dx\,,$$

   where A_n depends on the normalisation of the relevant orthogonal polynomial. This is **Parseval's Theorem** or **Parseval's Formula**, although this term is often reserved for the counterpart of this result in the case of the expansion of a periodic function $f(x)$ in a Fourier series (i.e., in a series of sine and cosine functions).

3. Consider the generating function of the Legendre polynomials,

$$F(t,x) = \frac{1}{(1-2xt+t^2)^{1/2}} = \sum_{n=0}^{\infty} P_n(x)\, t^n\,.$$

(a) Note that $(1-2xt+t^2)\,\dfrac{\partial F}{\partial t} = (x-t)\,F$. Use this to show that

$$n\,P_n(x) - (2n-1)\,x\,P_{n-1}(x) + (n-1)\,P_{n-2}(x) = 0\,.$$

(b) Similarly, $t\,\dfrac{\partial F}{\partial t} = (x-t)\,\dfrac{\partial F}{\partial x}$. Use this to show that

$$x\,\frac{dP_n(x)}{dx} - \frac{dP_{n-1}(x)}{dx} = n\,P_n(x)\,.$$

(c) Use the results above to show that

$$\frac{dP_n(x)}{dx} - x\,\frac{dP_{n-1}(x)}{dx} = n\,P_{n-1}(x)\,.$$

(d) Hence deduce that

$$\frac{dP_{n+1}(x)}{dx} - \frac{dP_{n-1}(x)}{dx} = (2n+1)\,P_n(x)\,,$$

$$(x^2-1)\,\frac{dP_n(x)}{dx} = n\,x\,P_n(x) - n\,P_{n-1}(x)\,,$$

$$(x^2-1)\,\frac{dP_n(x)}{dx} = -(n+1)\,x\,P_n(x) + (n+1)\,P_{n+1}(x)\,.$$

(e) Verify that

$$P_n(1) = 1\,, \quad P_n(-1) = (-1)^n\,, \quad P_{2n+1}(0) = 0\,, \quad P_{2n}(0) = \frac{(-1)^n\,(2n)!}{2^{2n}\,(n!)^2}\,.$$

4. Show that, if $m \geq n$ and $m-n$ is even,

$$\int_0^1 P_m(x)\,P_n(x)\,dx = \begin{cases} 0 & \text{if } m > n \\ (2n+1)^{-1} & \text{if } m = n\,. \end{cases}$$

5. Use the Rodrigues formula for $P_n(x)$ to show that

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

6. Consider the expansion in Legendre polynomials of a function $f(x)$ where $x \in (-1, 1)$:

$$f(x) = \sum_{n=0}^{\infty} (2n+1)\, f_n\, P_n(x).$$

Suppose $f(x) \in L_2(-1, 1)$. What is Parseval's formula in this case? What is the necessary condition on the asymptotic (that is, $n \to \infty$) behaviour of f_n?

7. The generating function of the Hermite polynomials is given by

$$e^{2tx - t^2} = \sum_{n=0}^{\infty} \frac{H_n(x)}{n!}\, t^n \,.$$

(a) Show that $\dfrac{dH_n(x)}{dx} = 2n\, H_{n-1}(x)$.

(b) Show that $H_{n+1}(x) - 2x\, H_n(x) + 2n\, H_{n-1}(x) = 0$.

(c) Hence show that $H_n(x)$ satisfies the Hermite equation

$$\frac{d^2\, H_n(x)}{dx^2} - 2x\, \frac{dH_n(x)}{dx} + 2n\, H_n(x) = 0\,.$$

(d) Establish the Rodrigues formula for Hermite polynomials, namely,

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

(e) Show that $H_{2n}(0) = \dfrac{(-1)^n\,(2n)!}{n!}$.

8. The generating function of the generalized Laguerre polynomials is given by

$$\frac{\exp\,[tx/(t-1)]}{(1-t)^{\alpha+1}} = \sum_{n=0}^{\infty} L_n^{\alpha}(x)\, t^n\,.$$

(a) Show that $L_n^{\alpha}(0) = \dfrac{\Gamma\,(n+\alpha+1)}{\Gamma(\alpha+1)\, n!}$.

(b) Show that $L_1^{\alpha}(x) = \alpha + 1 - x$.