

LAST TIME: Green functions

A few other examples of the use of special functions.

Quantum mechanical simple harmonic oscillator

The time-independent Schrodinger equation for the simple harmonic oscillator potential energy function is given by

$$-\frac{\hbar^2}{2m} \frac{d^2\psi}{dx^2} + \frac{1}{2} m\omega^2 x^2 \psi = E\psi.$$

You are probably aware that the wave function solution for the QSHO is the Hermite polynomial, but this equation is not quite in the correct form for that ODE. Therefore, we make the substitution given by $\xi = \alpha x \Rightarrow \frac{d}{dx} = \alpha \frac{d}{d\xi} \Rightarrow \frac{d^2}{dx^2} = \alpha^2 \frac{d^2}{d\xi^2}$. Making these substitutions into the Schrodinger equation and doing a bit of algebra gives

$$\frac{d^2\psi(\xi)}{d\xi^2} + \frac{2mE}{\hbar^2\alpha^2} \psi(\xi) - \frac{m^2\omega^2}{\hbar^2\alpha^4} \xi^2 \psi(\xi) = 0.$$

Now set $\frac{m^2\omega^2}{\hbar^2\alpha^4} = 1$ to get $\alpha^2 = \frac{m\omega}{\hbar}$ and $\xi = \sqrt{\frac{m\omega}{\hbar}} x$ with $\epsilon = \frac{2mE}{\hbar^2\alpha^2} = \frac{2E}{\hbar\omega}$.

Finally, the ODE is given by

$$\frac{d^2\psi(\xi)}{d\xi^2} + (\epsilon - \xi^2)\psi(\xi) = 0.$$

When $\xi \gg x$, we get an asymptotic solution to the equation which suggests that the general form of the solution could be written as

$$\psi(\xi) = u(\xi)e^{-\xi^2/2}.$$

Finally, this equation converts to

$$\frac{d^2u}{d\xi^2} - 2\xi \frac{du}{d\xi} + (\epsilon - 1)u = 0.$$

This equation is similar to the standard form of Hermite's ODE given by

$$\frac{d^2H}{d\xi^2} - 2\xi \frac{dH}{d\xi} + 2nH = 0,$$

where $H(\xi)$ are the Hermite polynomials. One important question is whether or not the value $2n = (\epsilon - 1)$ is an integer. We may solve this equation using the method of Frobenius as we have done before. Doing so, and requiring a normalizable solution requires that n be an integer so the series terminates as a polynomial. Therefore, we get $E = (n + 1/2)\hbar\omega$.

We may also set up the Schrodinger equation for a central force (or central potential) in spherical coordinates to get

$$-\frac{\hbar^2}{2m} \left[\frac{1}{r^2} \frac{\partial}{\partial r} \left(r^2 \frac{\partial}{\partial r} \right) + \frac{1}{r^2 \sin \theta} \frac{\partial}{\partial \theta} \left(\sin \theta \frac{\partial}{\partial \theta} \right) + \frac{1}{r^2 \sin^2 \theta} \frac{\partial^2}{\partial \phi^2} \right] \psi + V(r)\psi = E\psi.$$

As usual, we seek a solution in the form of separation of variables to obtain

$$\psi(r, \theta, \phi) = R(r)Y(\theta, \phi).$$

$$\begin{aligned} \frac{1}{r^2} \frac{\partial}{\partial r} \left(r^2 \frac{\partial}{\partial r} \right) R(r) Y(\theta, \phi) + \frac{1}{r^2 \sin \theta} \frac{\partial}{\partial \theta} \left(\sin \theta \frac{\partial}{\partial \theta} \right) R(r) Y(\theta, \phi) \\ + \frac{1}{r^2 \sin^2 \theta} \frac{\partial^2}{\partial \phi^2} R(r) Y(\theta, \phi) - \frac{2m}{\hbar^2} [V(r) - E] R(r) Y(\theta, \phi) = 0 \\ \Rightarrow Y(\theta, \phi) \frac{1}{r^2} \frac{\partial}{\partial r} \left(r^2 \frac{\partial}{\partial r} \right) R(r) + R(r) \frac{1}{r^2 \sin \theta} \frac{\partial}{\partial \theta} \left(\sin \theta \frac{\partial}{\partial \theta} \right) Y(\theta, \phi) \\ + R(r) \frac{1}{r^2 \sin^2 \theta} \frac{\partial^2}{\partial \phi^2} Y(\theta, \phi) - \frac{2m}{\hbar^2} [V(r) - E] R(r) Y(\theta, \phi) = 0. \end{aligned}$$

Dividing the equation by $R(r)Y(\theta, \phi)$, multiplying by r^2 , and rearranging terms, this becomes

$$\begin{aligned} \left\{ \frac{1}{R(r)} \frac{\partial}{\partial r} \left(r^2 \frac{\partial}{\partial r} \right) R(r) - \frac{2mr^2}{\hbar^2} [V(r) - E] \right\} \\ + \left[\frac{1}{Y(\theta, \phi) \sin \theta} \frac{\partial}{\partial \theta} \left(\sin \theta \frac{\partial}{\partial \theta} \right) Y(\theta, \phi) + \frac{1}{Y(\theta, \phi) \sin^2 \theta} \frac{\partial^2}{\partial \phi^2} Y(\theta, \phi) \right] = 0. \end{aligned}$$

We may choose the separation constant to be K , but the work of mathematicians and physicists has shown that it is better to choose $\ell(\ell + 1)$. Then,

$$\frac{1}{R(r)} \frac{d}{dr} \left(r^2 \frac{d}{dr} \right) R(r) - \frac{2mr^2}{\hbar^2} [V(r) - E] = \ell(\ell + 1)$$

and

$$\frac{1}{Y(\theta, \phi) \sin \theta} \frac{\partial}{\partial \theta} \left(\sin \theta \frac{\partial}{\partial \theta} \right) Y(\theta, \phi) + \frac{1}{Y(\theta, \phi) \sin^2 \theta} \frac{\partial^2}{\partial \phi^2} Y(\theta, \phi) = -\ell(\ell + 1),$$

where the radial component and angular components have been separated. These are the same spherical harmonics we have dealt with before, and we could have gone about this by using separate functions for θ and ϕ as we did before. The solution to the radial equation yields a set of Laguerre polynomials (not an orthonormal set) as well as a set of Laguerre functions that are.

An interesting observation is that mathematicians knew about the ODEs that we use long before we put the physics into these equations. You will see much more about these operations in quantum mechanics.

Let's consider the wave equation without sources in spherical coordinates given by

$$\nabla^2\psi - \frac{1}{c^2} \frac{\partial^2\psi}{\partial t^2} = 0.$$

As I pointed out earlier, we may assume a time dependence of $e^{i\omega t}$ to obtain the Helmholtz equation and separate variables again. The separation gives the ϕ - term as $\exp(im\phi)$, the θ - term as associate Legendre functions of the first and second kind, and the radial equation is given by

$$\frac{1}{R} \frac{\partial}{\partial r} \left(r^2 \frac{\partial R}{\partial r} \right) + k^2 r^2 R - \ell(\ell + 1)R = 0.$$

The solution to this equation is given by $R(r) = \frac{J_{\ell+1/2}(kr)}{\sqrt{r}}$, which is a spherical Bessel function, as opposed to the cylindrical Bessel functions we studied in connection with Laplace's equation for cylindrical geometries. The complete solution for the wave equation without sources in spherical coordinates is given by

$$\psi(r, \theta, \phi, t) = j_\ell(kr) P_\ell^m(\theta) e^{im\phi} e^{-ikct}.$$

Spherical Hankel functions of the first and second kind are defined in the same way as they were for cylindrical functions. Because the equation for spherical Bessel functions are Sturm-Liouville equations, they also form a complete set of orthogonal functions. You will see these spherical Hankel functions and spherical Bessel functions when you study the wave equation with sources to learn about radiation. I will return to the wave equation with sources after we study applications of the residue theorem.

NEXT TIME: Complex analysis