

SPHERICALLY SYMMETRIC POTENTIALS: HERMITICITY OF THE RADIAL FUNCTION

Link to: physicspages home page.

To leave a comment or report an error, please use the auxiliary blog.

Shankar, R. (1994), *Principles of Quantum Mechanics*, Plenum Press. Chapter 12, Exercise 12.6.3.

[If some equations are too small to read easily, use your browser's magnifying option (Ctrl + on Chrome, probably something similar on other browsers).]

The Schrödinger equation in 3-d for a potential that depends only on r is

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

Eigenfunctions in this equation satisfy

$$\psi = R_{Elm}(r) Y_l^m(\theta, \phi) \quad (2)$$

where the subscript Elm refers to the energy E and the angular momentum quantum numbers l and m . Y_l^m is a spherical harmonic and R_{Elm} is the radial function which depends on the potential V . With the substitution

$$R_{El}(r) = \frac{U_{El}(r)}{r} \quad (3)$$

the differential equation reduces to

$$\left[-\frac{\hbar^2}{2\mu} \frac{d^2}{dr^2} + V(r) + \frac{l(l+1)\hbar^2}{2\mu r^2} \right] U_{El} = EU_{El} \quad (4)$$

The quantity in the square brackets is an operator which will call $D_l(r)$:

$$D_l(r) \equiv -\frac{\hbar^2}{2\mu} \frac{d^2}{dr^2} + V(r) + \frac{l(l+1)\hbar^2}{2\mu r^2} \quad (5)$$

Equation 4 is similar to the 1-d Schrödinger equation except that the variable r goes from 0 to ∞ rather than from $-\infty$ to ∞ , and the potential is modified by the 'centrifugal term' $\frac{l(l+1)\hbar^2}{2\mu r^2}$. Because r begins at 0 rather than $-\infty$, the usual boundary conditions on U (that it tend to zero at $\pm\infty$) must also be modified. We can get the new boundary conditions by imposing the hermiticity condition, which says that

$$\int_0^\infty U_1^* (D_l U_2) dr = \left[\int_0^\infty U_2^* (D_l U_1) dr \right]^* \quad (6)$$

$$= \int_0^\infty (D_l U_1)^* U_2 dr \quad (7)$$

The two terms $V(r) + \frac{l(l+1)\hbar^2}{2\mu r^2}$ in 5 are real and multiplicative, so the hermiticity condition is automatically satisfied for them. For the derivative term, we can use the usual integration by parts.

$$\int_0^\infty U_1^* \left(\frac{d^2}{dr^2} U_2 \right) dr = U_1^* \frac{dU_2}{dr} \Big|_0^\infty - \int_0^\infty \frac{dU_1^*}{dr} \frac{dU_2}{dr} dr \quad (8)$$

$$= U_1^* \frac{dU_2}{dr} \Big|_0^\infty - U_2 \frac{dU_1^*}{dr} \Big|_0^\infty + \int_0^\infty U_2 \left(\frac{d^2}{dr^2} U_1^* \right) dr \quad (9)$$

If we require

$$U_1^* \frac{dU_2}{dr} \Big|_0^\infty - U_2 \frac{dU_1^*}{dr} \Big|_0^\infty = 0 \quad (10)$$

then we have

$$\int_0^\infty U_1^* \left(\frac{d^2}{dr^2} U_2 \right) dr = \int_0^\infty U_2 \left(\frac{d^2}{dr^2} U_1^* \right) dr \quad (11)$$

$$= \left[\int_0^\infty U_2^* \left(\frac{d^2}{dr^2} U_1 \right) dr \right]^* \quad (12)$$

and the hermiticity condition 6 is satisfied.

PINGBACKS

Pingback: nondegenerate states in 3-d: spherically symmetric systems

Pingback: free particle in spherical coordinates: finding the solutions

Pingback: radial function for large r

Pingback: radial function for small r

Pingback: Free particle in spherical coordinates