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

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

Eigenfunctions in this equation satisfy

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

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

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

the differential equation reduces to

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

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

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

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

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

$$= \int_0^\infty \left(D_l U_1\right)^* U_2 dr \tag{7}$$

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.

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

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

If we require

$$U_1^*\frac{dU_2}{dr}\bigg|_0^\infty - U_2\frac{dU_1^*}{dr}\bigg|_0^\infty = 0 \tag{10}$$

then we have

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

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

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