

Energy Eigenproblem in Two Dimensions

In one dimension, the energy eigenproblem is

$$-\frac{\hbar^2}{2m} \frac{d^2\eta(x)}{dx^2} + V(x)\eta(x) = E\eta(x). \quad (1)$$

The generalization to two dimensions is straightforward:

$$-\frac{\hbar^2}{2m} \left[\frac{\partial^2\eta(x, y)}{\partial x^2} + \frac{\partial^2\eta(x, y)}{\partial y^2} \right] + V(x, y)\eta(x, y) = E\eta(x, y). \quad (2)$$

The part in square brackets is called “the Laplacian of $\eta(x, y)$ ” and represented by the symbol “ ∇^2 ” as follows

$$\left[\frac{\partial^2\eta(x, y)}{\partial x^2} + \frac{\partial^2\eta(x, y)}{\partial y^2} \right] \equiv \nabla^2\eta(x, y). \quad (3)$$

Thus the “mathematical form” of the energy eigenproblem is

$$\nabla^2\eta(\vec{r}) = -\frac{2m}{\hbar^2} [E - V(\vec{r})]\eta(\vec{r}). \quad (4)$$

Suppose $V(x, y)$ is a function of distance from the origin r only. Then it makes sense to use polar coordinates r and θ rather than Cartesian coordinates x and y . What is the expression for the Laplacian in polar coordinates? This can be uncovered through the chain rule, and it’s pretty hard to do. Fortunately, you can look up the answer:

$$\nabla^2\eta(\vec{r}) = \left[\frac{1}{r} \frac{\partial}{\partial r} \left(r \frac{\partial\eta(r, \theta)}{\partial r} \right) + \frac{1}{r^2} \frac{\partial^2\eta(r, \theta)}{\partial\theta^2} \right]. \quad (5)$$

Thus, the partial differential equation to be solved is

$$\left[\frac{1}{r} \frac{\partial}{\partial r} \left(r \frac{\partial\eta(r, \theta)}{\partial r} \right) + \frac{1}{r^2} \frac{\partial^2\eta(r, \theta)}{\partial\theta^2} \right] = -\frac{2m}{\hbar^2} [E - V(r)]\eta(r, \theta). \quad (6)$$

As before, this is a linear partial differential equation, so we’ll cast around for solutions knowing that a linear combination of solutions will also be a solution. We cast around through the technique of “separation of variables”, namely by looking for solutions of the form

$$\eta(r, \theta) = R(r)\Theta(\theta). \quad (7)$$

Plugging this form into the PDE gives

$$\left[\frac{1}{r} \Theta(\theta) \frac{d}{dr} (rR'(r)) + \frac{1}{r^2} R(r) \Theta''(\theta) \right] = -\frac{2m}{\hbar^2} [E - V(r)] R(r) \Theta(\theta) \quad (8)$$

whence

$$\frac{r \frac{d}{dr} (rR'(r))}{R(r)} + \frac{\Theta''(\theta)}{\Theta(\theta)} = -\frac{2m}{\hbar^2} r^2 [E - V(r)] \quad (9)$$

and, separating the variables,

$$\frac{r \frac{d}{dr} (rR'(r))}{R(r)} + \frac{2m}{\hbar^2} r^2 [E - V(r)] = -\frac{\Theta''(\theta)}{\Theta(\theta)} = \text{const.} \quad (10)$$

In the usual separation-of-variables argument, we recognize that if a function of r alone is equal to a function of θ alone, where r and θ are independent variables, then both functions must be equal to the same constant.

First, we look at the angular part:

$$\Theta''(\theta) = -\text{const}\Theta(\theta). \quad (11)$$

This is the differential equation for a mass on a spring! The two linearly independent solutions are

$$\Theta(\theta) = \sin(\sqrt{\text{const}} \theta) \quad \text{or} \quad \Theta(\theta) = \cos(\sqrt{\text{const}} \theta). \quad (12)$$

Now, the boundary condition for this ODE is just that the function must come back to itself if θ increases by 2π :

$$\Theta(\theta) = \Theta(2\pi + \theta). \quad (13)$$

If you think about this for a minute, you'll see that this means $\sqrt{\text{const}}$ must be an integer. The negative integers don't give us anything new, so we'll take

$$\sqrt{\text{const}} = \ell \quad \text{where} \quad \ell = 0, 1, 2, \dots \quad (14)$$

In summary, the solution to the angular problem is

$$\begin{array}{ccccccc} \ell = 0 & \ell = 1 & \ell = 2 & \ell = 3 & \dots & & \\ \Theta(\theta) & 1 & \sin \theta \text{ or } \cos \theta & \sin 2\theta \text{ or } \cos 2\theta & \sin 3\theta \text{ or } \cos 3\theta & \dots & \end{array}$$

Now we move on to the radial part of the problem:

$$\frac{r \frac{d}{dr} (rR'(r))}{R(r)} + \frac{2m}{\hbar^2} r^2 [E - V(r)] = \text{const} = \ell^2. \quad (15)$$

or

$$\begin{aligned} \frac{r \frac{d}{dr} (rR'(r))}{R(r)} &= -\frac{2m}{\hbar^2} r^2 [E - V(r)] + \ell^2 \\ \frac{r \frac{d}{dr} (rR'(r))}{R(r)} &= -\frac{2m}{\hbar^2} r^2 \left[E - V(r) - \frac{\hbar^2}{2mr^2} \ell^2 \right] \\ \frac{1}{r} \frac{d}{dr} (rR'(r)) &= -\frac{2m}{\hbar^2} \left[E - V(r) - \frac{\hbar^2}{2mr^2} \ell^2 \right] R(r) \end{aligned} \quad (16)$$

I've set up the problem in this form to compare it with the one-dimensional energy eigenproblem,

$$\frac{d^2 \eta(x)}{dx^2} = -\frac{2m}{\hbar^2} [E - V(x)] \eta(x). \quad (17)$$

You see that the right-hand sides are vaguely similar but the left-hand sides are not. The following trick makes the left-hand sides more similar:

$$\text{If } u(r) = \sqrt{r}R(r), \quad \text{then } \frac{1}{r} \frac{d}{dr} (rR'(r)) = \frac{1}{\sqrt{r}} \left(u''(r) + \frac{1}{4} \frac{u(r)}{r^2} \right). \quad (18)$$

Using this change of function, the radial equation (16) becomes

$$u''(r) = -\frac{2m}{\hbar^2} \left[E - V(r) - \frac{\hbar^2(\ell + \frac{1}{2})(\ell - \frac{1}{2})}{2m} \frac{1}{r^2} \right] u(r), \quad (19)$$

In this form, the radial equation is exactly like a one-dimensional energy eigenproblem, except that where the one-dimensional problem has the function $V(x)$, the radial problem has the function

$$V(r) + \hbar^2(\ell + \frac{1}{2})(\ell - \frac{1}{2})/2mr^2.$$

These two functions play similar mathematical roles in the two problems. To emphasize these similar roles, we define an “effective potential energy” for the radial problem, namely

$$V_{\text{eff}}(r) = V(r) + \frac{\hbar^2(\ell + \frac{1}{2})(\ell - \frac{1}{2})}{2m} \frac{1}{r^2}. \quad (20)$$

Don’t read too much into the term “effective potential energy.” No actual potential energy will depend upon the particle’s mass, or on \hbar , or on the separation constant ℓ ! I’m not saying that $V_{\text{eff}}(r)$ is a potential energy function, merely that it plays the mathematical role of one in solving this eigenproblem.

Now that the radial equation (19) is in exact correspondence with the one-dimensional equation (17), we can solve this eigenproblem using the same “curve toward or away from axis” techniques that we’ve already developed for the one-dimensional problem. (Or any other technique which works for the one-dimensional problem.) The resulting eigenfunctions and eigenvalues will, of course, depend upon the value of the separation constant ℓ , because the effective potential depends upon the value of ℓ . And as always, for each ℓ there will be many eigenvalues and eigenfunctions, which we will label by index $n = 1, 2, 3, \dots$ calling them $u_{n,\ell}(r)$ with eigenvalue $E_{n,\ell}$.

Summary:

To solve the two-dimensional energy eigenproblem

$$-\frac{\hbar^2}{2m} \nabla^2 \eta(\vec{r}) - V(r)\eta(\vec{r}) = E\eta(\vec{r}), \quad (21)$$

first solve the radial energy eigenproblem

$$-\frac{\hbar^2}{2m} \frac{du(r)}{dr} + \left[V(r) + \frac{\hbar^2(\ell + \frac{1}{2})(\ell - \frac{1}{2})}{2m} \frac{1}{r^2} \right] u(r) = Eu(r) \quad (22)$$

for $\ell = 0, 1, 2, \dots$. For a given ℓ , call the resulting energy eigenfunctions and eigenvalues $u_{n,\ell}(r)$ and $E_{n,\ell}$ for $n = 1, 2, 3, \dots$. Then the two-dimensional solutions are

$$\text{For } \ell = 0: \quad \eta(r, \theta) = \frac{u_{n,0}(r)}{\sqrt{r}} \quad \text{with energy } E_{n,0} \quad (23)$$

and

$$\text{For } \ell = 1, 2, 3, \dots: \quad \eta(r, \theta) = \frac{u_{n,\ell}(r)}{\sqrt{r}} \sin(\ell\theta) \quad \text{and} \quad \eta(r, \theta) = \frac{u_{n,\ell}(r)}{\sqrt{r}} \cos(\ell\theta) \quad \text{with energy } E_{n,\ell}. \quad (24)$$