Problem 2.1

Prove the following three theorems:

(a) For normalizable solutions, the separation constant E must be *real*. *Hint:* Write E (in Equation 2.7) as $E_0 + i\Gamma$ (with E_0 and Γ real), and show that if Equation 1.20 is to hold for all t, Γ must be zero.

(b) The time-independent wave function $\psi(x)$ can always be taken to be *real* (unlike $\Psi(x,t)$, which is necessarily complex). This doesn't mean that every solution to the time-independent Schrödinger *is* real; what it says is that if you've got one that is *not*, it can always be expressed as a linear combination of solutions (with the same energy) that *are*. So you *might as well* stick to ψs that are real. *Hint:* If $\psi(x)$ satisfies Equation 2.5, for a given E, so too does its complex conjugate, and hence also the real linear combinations $(\psi + \psi^*)$ and $i(\psi - \psi^*)$.

(c) If $V(x)$ is an **even function** (that is, $V(-x) = V(x)$) then $\psi(x)$ can always be taken to be either even or odd. *Hint:* If $\psi(x)$ satisfies Equation 2.5, for a given E, so too does $\psi(-x)$, and hence also the even and odd linear combinations $\psi(x) \pm \psi(-x)$.

[TYPO: "Are" should be "is."]

Solution

The governing equation for the wave function is the Schrödinger equation.

$$i\hbar\frac{\partial\Psi}{\partial t} = -\frac{\hbar^2}{2m}\frac{\partial^2\Psi}{\partial x^2} + V(x,t)\Psi(x,t)$$

Because it's linear and homogeneous, the method of separation of variables can be applied to try and solve it: Assume a product solution of the form $\Psi(x,t) = \psi(x)\phi(t)$ and plug it into the equation.

$$i\hbar\frac{\partial}{\partial t}[\psi(x)\phi(t)] = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}[\psi(x)\phi(t)] + V(x,t)[\psi(x)\phi(t)]$$

Evaluate the derivatives.

$$i\hbar\psi(x)\phi'(t) = -\frac{\hbar^2}{2m}\psi''(x)\phi(t) + V(x,t)\psi(x)\phi(t)$$

Divide both sides by $\psi(x)\phi(t)$.

$$i\hbar\frac{\phi'(t)}{\phi(t)} = -\frac{\hbar^2}{2m}\frac{\psi''(x)}{\psi(x)} + V(x,t)$$

For the special case that the potential energy V is independent of time, the left side is only a function of t, and the right side is only a function of x. Consequently, both functions must be equal to a constant E.

$$i\hbar\frac{\phi'(t)}{\phi(t)} = -\frac{\hbar^2}{2m}\frac{\psi''(x)}{\psi(x)} + V(x) = E$$

As a result of applying the method of separation of variables, Schrödinger's equation has reduced to two ODEs—one in each of the independent variables, x and t.

$$\left.\begin{aligned} i\hbar\frac{\phi'(t)}{\phi(t)} &= E \\ -\frac{\hbar^2}{2m}\frac{\psi''(x)}{\psi(x)} + V(x) &= E \end{aligned}\right\}$$

Values of E for which the boundary conditions of this second equation are satisfied are known as eigenvalues (or eigenenergies in this context), and the nontrivial solutions $\psi(x)$ that satisfy this second equation are known as eigenfunctions (or eigenstates in this context). The left side of the first equation can be written as the derivative of a logarithm by the chain rule.

$$i\hbar\frac{d}{dt}\ln\phi(t) = E$$

$$\frac{d}{dt}\ln\phi(t) = -\frac{iE}{\hbar}$$

Integrate both sides with respect to t.

$$\ln\phi(t) = -\frac{iE}{\hbar}t + C$$

Exponentiate both sides.

$$\begin{aligned} \phi(t) &= e^{-iEt/\hbar + C} \\ &= e^{-iEt/\hbar}e^C \end{aligned}$$

Use a new constant A for e^C.

$$\phi(t) = Ae^{-iEt/\hbar}$$

Therefore, the product solution so far is $\Psi(x,t) = A\psi(x)e^{-iEt/\hbar}$. This constant A is due to the fact that the Schrödinger equation is homogeneous.

Part (a)

Suppose that E has an imaginary component: $E = E_0 + i\Gamma$.

$$\begin{aligned} \Psi(x,t) &= A\psi(x)e^{-i(E_0+i\Gamma)t/\hbar} \\ &= A\psi(x)e^{-iE_0t/\hbar}e^{\Gamma t/\hbar} \end{aligned}$$

Since the wave function is normalizable, the integral of $|\Psi(x,t)|^2$ over the whole line must be 1.

$$\begin{aligned} 1 &= \int_{-\infty}^{\infty} |\Psi(x,t)|^2\,dx \\ &= \int_{-\infty}^{\infty} \Psi(x,t)\Psi^*(x,t)\,dx \\ &= \int_{-\infty}^{\infty} [A\psi(x)e^{-iE_0t/\hbar}e^{\Gamma t/\hbar}][A\psi(x)e^{-iE_0t/\hbar}e^{\Gamma t/\hbar}]^*\,dx \\ &= \int_{-\infty}^{\infty} [A\psi(x)e^{-iE_0t/\hbar}e^{\Gamma t/\hbar}][A^*\psi^*(x)e^{iE_0t/\hbar}e^{\Gamma t/\hbar}]\,dx \\ &= e^{2\Gamma t/\hbar}\int_{-\infty}^{\infty} |A|^2|\psi(x)|^2\,dx \end{aligned}$$

This integral wipes out x, resulting in a constant. In order for equality to be maintained, it's necessary that $\Gamma = 0$. Therefore, E is real.

Part (b)

Consider a complex function $f(z)$ with a real part Re $f(z)$ and an imaginary part Im $f(z)$, both of which are real.

$$f(z) = \text{Re } f(z) + i \,\text{Im } f(z)$$
$$f^*(z) = \text{Re } f(z) - i \,\text{Im } f(z)$$

Adding the respective sides of these two equations yields

$$f(z) + f^*(z) = 2 \,\text{Re } f(z) \qquad \rightarrow \qquad \text{Re } f(z) = \frac{f(z) + f^*(z)}{2},$$

whereas subtracting the respective sides of these two equations yields

$$f(z) - f^*(z) = 2i \,\text{Im } f(z) \qquad \rightarrow \qquad \text{Im } f(z) = \frac{f(z) - f^*(z)}{2i}.$$

Multiply both sides of the ODE in x by $\psi(x)$.

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} + [V(x) - E]\psi(x) = 0$$

Take the complex conjugate of both sides.

$$-\frac{\hbar^2}{2m}\frac{d^2\psi^*}{dx^2} + [V(x) - E]\psi^*(x) = 0$$

Both ψ and ψ^* satisfy the same ODE; the general solution for it is then a linear combination of the two because the ODE is linear.

$$C_1\psi(x) + C_2\psi^*(x)$$

By taking $C_1 = 1/2$ and $C_2 = 1/2$ [or $C_1 = 1/(2i)$ and $C_2 = -1/(2i)$], a real function can be obtained for the solution.

Part (c)

Multiply both sides of the ODE in x by $\psi(x)$.

$$-\frac{\hbar^2}{2m}\frac{d^2\psi(x)}{dx^2} + [V(x) - E]\psi(x) = 0$$

Make the substitution $x = -s$.

$$-\frac{\hbar^2}{2m}\frac{d^2\psi(-s)}{dx^2} + [V(-s) - E]\psi(-s) = 0 \tag{1}$$

Use the chain rule to write the derivative in terms of this new variable.

$$\frac{d\psi}{dx} = \frac{d\psi}{ds}\frac{ds}{dx} = \frac{d\psi}{ds}(-1) = -\frac{d\psi}{ds}$$

$$\frac{d^2\psi}{dx^2} = \frac{d}{dx}\left(\frac{d\psi}{dx}\right) = \frac{ds}{dx}\frac{d}{ds}\left(-\frac{d\psi}{ds}\right) = (-1)\frac{d}{ds}\left(-\frac{d\psi}{ds}\right) = \frac{d^2\psi}{ds^2}$$

Consequently, equation (1) becomes

$$-\frac{\hbar^2}{2m}\frac{d^2\psi(-s)}{ds^2} + [V(-s) - E]\psi(-s) = 0.$$

s is just a dummy variable and can be replaced by x.

$$-\frac{\hbar^2}{2m}\frac{d^2\psi(-x)}{dx^2} + [V(-x) - E]\psi(-x) = 0$$

If V is an even function, then $V(-x) = V(x)$

$$-\frac{\hbar^2}{2m}\frac{d^2\psi(-x)}{ds^2} + [V(x) - E]\psi(-x) = 0$$

and both $\psi(x)$ and $\psi(-x)$ satisfy the ODE in x. The general solution is then a linear combination of these two by the superposition principle.

$$C_3\psi(x) + C_4\psi(-x)$$

It can be made even by selecting $C_3 = 1$ and $C_4 = 1$, for example, and it can be made odd by selecting $C_3 = 1$ and $C_4 = -1$.