Problem 2.39

In Problem 2.7(d) you got the expectation value of the energy by summing the series in Equation 2.21, but I warned you (in footnote 21) not to try it the "old fashioned way," $\langle H\rangle = \int \Psi(x,0)^* \hat{H}\Psi(x,0)\,dx$, because the discontinuous first derivative of $\Psi(x,0)$ renders the second derivative problematic. Actually, you *could* have done it using integration by parts, but the Dirac delta function affords a much cleaner way to handle such anomalies.

(a) Calculate the first derivative of $\Psi(x,0)$ (in Problem 2.7), and express the answer in terms of the step function, $\theta(x-a/2)$, defined in Equation 2.146.

(b) Exploit the result of Problem 2.23(b) to write the second derivative of $\Psi(x,0)$ in terms of the delta function.

(c) Evaluate the integral $\int \Psi(x,0)^* \hat{H}\Psi(x,0)\,dx$, and check that you get the same answer as before.

Solution

The normalized initial wave function in Problem 2.7 is for a particle in the infinite square well.

$$\Psi(x,0) = \begin{cases} Ax & \text{if } 0 \le x \le a/2 \\ A(a-x) & \text{if } a/2 \le x \le a \end{cases}$$

Calculate its first derivative with respect to x, expressing the result in terms of the Heaviside function $\theta(x)$.

$$\begin{aligned} \frac{d}{dx}\Psi(x,0) = \begin{cases} A & \text{if } 0 \le x \le a/2 \\ -A & \text{if } a/2 \le x \le a \end{cases} &= A\left[\theta(x) - \theta\left(x-\frac{a}{2}\right)\right] - A\left[\theta\left(x-\frac{a}{2}\right) - \theta(x-a)\right] \\ &= A\theta(x) - 2A\theta\left(x-\frac{a}{2}\right) + A\theta(x-a) \\ &= A\left[\theta(x) - 2\theta\left(x-\frac{a}{2}\right) + \theta(x-a)\right] \end{aligned}$$

Calculate its second derivative with respect to x, using the fact that $d\theta/dx = \delta(x)$, the Dirac delta function.

$$\begin{aligned} \frac{d^2}{dx^2}\Psi(x,0) &= A\left[\theta'(x) - 2\theta'\left(x-\frac{a}{2}\right) + \theta'(x-a)\right] \\ &= A\left[\delta(x) - 2\delta\left(x-\frac{a}{2}\right) + \delta(x-a)\right] \end{aligned}$$

In Problem 2.7 the normalization constant was found to be

$$A = 2\sqrt{\frac{3}{a^3}},$$

which means

$$\frac{d^2}{dx^2}\Psi(x,0) = 2\sqrt{\frac{3}{a^3}}\left[\delta(x) - 2\delta\left(x-\frac{a}{2}\right) + \delta(x-a)\right].$$

Now calculate the expectation value of energy at $t = 0$, noting that the potential energy is zero inside $0 \le x \le a$ and that $\Psi(x, 0)$ is zero outside $0 \le x \le a$.

$$\begin{aligned}
\langle E \rangle &= \int_{-\infty}^{\infty} \Psi^*(x,0)\hat{H}\Psi(x,0)\,dx \\
&= \int_0^a \Psi^*(x,0)\hat{H}\Psi(x,0)\,dx \\
&= \int_0^a \Psi^*(x,0)\left(\frac{\hat{p}^2}{2m} + 0\right)\Psi(x,0)\,dx \\
&= \frac{1}{2m}\int_0^a \Psi^*(x,0)\hat{p}^2\Psi(x,0)\,dx \\
&= \frac{1}{2m}\int_0^a \Psi^*(x,0)\left(-i\hbar\frac{\partial}{\partial x}\right)^2\Psi(x,0)\,dx \\
&= \frac{1}{2m}\int_0^a \Psi^*(x,0)\left(-\hbar^2\frac{\partial^2}{\partial x^2}\right)\Psi(x,0)\,dx \\
&= -\frac{\hbar^2}{2m}\int_0^a \Psi^*(x,0)\frac{d^2}{dx^2}\Psi(x,0)\,dx \\
&= -\frac{\hbar^2}{2m}\left\{\int_0^{a/2}\left(2\sqrt{\frac{3}{a^3}}x\right)2\sqrt{\frac{3}{a^3}}\left[\delta(x) - 2\delta\left(x-\frac{a}{2}\right) + \delta(x-a)\right]dx\right. \\
&\qquad\qquad \left. + \int_{a/2}^a\left[2\sqrt{\frac{3}{a^3}}(a-x)\right]2\sqrt{\frac{3}{a^3}}\left[\delta(x) - 2\delta\left(x-\frac{a}{2}\right) + \delta(x-a)\right]dx\right\} \\
&= -\frac{\hbar^2}{m}\sqrt{\frac{3}{a^3}}\left\{\int_0^{a/2} 2\sqrt{\frac{3}{a^3}}\left[\overbrace{x\delta(x)}^{=\,0} - 2x\delta\left(x-\frac{a}{2}\right) + \cancel{x\delta(x-a)}\right]dx\right. \\
&\qquad\qquad \left. + \int_{a/2}^a 2\sqrt{\frac{3}{a^3}}\left[\cancel{(a-x)\delta(x)} - 2(a-x)\delta\left(x-\frac{a}{2}\right) + \underbrace{(a-x)\delta(x-a)}_{=\,0}\right]dx\right\} \\
&= -\frac{\hbar^2}{m}\sqrt{\frac{3}{a^3}}\left\{-2\int_0^{a/2}\left(2\sqrt{\frac{3}{a^3}}x\right)\delta\left(x-\frac{a}{2}\right)dx\right. \\
&\qquad\qquad \left. - 2\int_{a/2}^a\left[2\sqrt{\frac{3}{a^3}}(a-x)\right]\delta\left(x-\frac{a}{2}\right)dx\right\} \\
&= \frac{2\hbar^2}{m}\sqrt{\frac{3}{a^3}}\left\{\int_0^{a/2}\left(2\sqrt{\frac{3}{a^3}}x\right)\delta\left(x-\frac{a}{2}\right)dx + \int_{a/2}^a\left[2\sqrt{\frac{3}{a^3}}(a-x)\right]\delta\left(x-\frac{a}{2}\right)dx\right\} \\
&= \frac{2\hbar^2}{m}\sqrt{\frac{3}{a^3}}\int_0^a \Psi(x,0)\delta\left(x-\frac{a}{2}\right)dx \\
&= \frac{2\hbar^2}{m}\sqrt{\frac{3}{a^3}}\,\Psi\left(\frac{a}{2},0\right) \\
&= \frac{2\hbar^2}{m}\sqrt{\frac{3}{a^3}}\left(2\sqrt{\frac{3}{a^3}}\frac{a}{2}\right) = \frac{6\hbar^2}{ma^2}
\end{aligned}$$