the coefficients f_n in the Fourier series

$$\psi(x,0) = \sum_{n=1}^{\infty} f_n \sqrt{\frac{2}{L}} \sin\left(\frac{\pi n x}{L}\right) \tag{2.82}$$

are the inner products

$$f_n = \langle n|\psi,0\rangle = \int_0^L dx \sqrt{\frac{2}{L}} \sin\left(\frac{\pi n x}{L}\right) \psi(x,0). \tag{2.83}$$

They are proportional to $1/n$ in accord with (2.58)

$$f_n = \frac{2}{L} \int_{L/4}^{3L/4} dx \sin\left(\frac{\pi n x}{L}\right) = \frac{2}{\pi n} \left[\cos\left(\frac{\pi n}{4}\right) - \cos\left(\frac{3\pi n}{4}\right)\right]. \tag{2.84}$$

Figure 2.5 plots the square wave function $\psi(x,0)$ (2.80, straight solid lines) and its 10-term (solid curve) and 100-term (dashes) Fourier series (2.82) for an interval of length $L = 2$. Gibbs's overshoot reaches 1.093 at $x = 0.52$ for 100 terms and 1.0898 at $x = 0.502$ for 1000 terms (not shown), amounting to about 9% of the unit discontinuity at $x = 1/2$. A similar overshoot occurs at $x = 3/2$.

How does $\psi(x,0)$ evolve with time? Since $\psi_n(x)$, the Fourier component (2.77), is an eigenfunction of H with energy E_n, the time-evolution operator $U(t) = \exp(-iHt/\hbar)$ takes $\psi(x,0)$ into

$$\psi(x,t) = e^{-iHt/\hbar}\,\psi(x,0) = \sum_{n=1}^{\infty} f_n \sqrt{\frac{2}{L}} \sin\left(\frac{\pi n x}{L}\right) e^{-iE_n t/\hbar}. \tag{2.85}$$

Because $E_n = (n\pi\hbar/L)^2/2m$, the wave function at time t is

$$\psi(x,t) = \sum_{n=1}^{\infty} f_n \sqrt{\frac{2}{L}} \sin\left(\frac{\pi n x}{L}\right) e^{-i\hbar(n\pi)^2 t/(2mL^2)}. \tag{2.86}$$

It is awkward to plot complex functions, so Fig. 2.6 displays the probability distributions $P(x,t) = |\psi(x,t)|^2$ of the 1000-term Fourier series (2.86) for the wave function $\psi(x,t)$ at $t = 0$ (thick curve), $t = 10^{-3}\,\tau$ (medium curve), and $\tau = 2mL^2/\hbar$ (thin curve). The discontinuities in the initial wave function $\psi(x,0)$ cause both the Gibbs overshoots at $x = 1/2$ and $x = 3/2$ seen in the series for $\psi(x,0)$ plotted in Fig. 2.5 and the choppiness of the probability distribution $P(x,t)$ exhibited in Fig.(2.6). □

Example 2.11 (Time Evolution of a Continuous Function) What does the Fourier series of a continuous function look like? How does it evolve