Problem 2.61

One way to obtain the allowed energies of a potential well numerically is to turn the Schrödinger equation into a *matrix* equation, by discretizing the variable x. Slice the relevant interval at evenly spaced points $\{x_j\}$, with $x_{j+1} - x_j \equiv \Delta x$, and let $\psi_j \equiv \psi(x_j)$ (likewise $V_j \equiv V(x_j)$). Then

$$\frac{d\psi}{dx} \approx \frac{\psi_{j+1} - \psi_j}{\Delta x}, \ \frac{d^2\psi}{dx^2} \approx \frac{(\psi_{j+1} - \psi_j) - (\psi_j - \psi_{j-1})}{(\Delta x)^2} = \frac{\psi_{j+1} - 2\psi_j + \psi_{j-1}}{(\Delta x)^2}. \tag{2.195}$$

(The approximation presumably improves as Δx decreases.) The discretized Schrödinger equation reads

$$-\frac{\hbar^2}{2m}\left(\frac{\psi_{j+1} - 2\psi_j + \psi_{j-1}}{(\Delta x)^2}\right) + V_j\psi_j = E\psi_j, \tag{2.196}$$

or

$$-\lambda\psi_{j+1} + (2\lambda + V_j)\,\psi_j - \lambda\psi_{j-1} = E\psi_j, \quad \text{where} \quad \lambda \equiv \frac{\hbar^2}{2m\,(\Delta x)^2}. \tag{2.197}$$

In matrix form,

$$\mathsf{H}\Psi = E\Psi \tag{2.198}$$

where (letting $v_j \equiv V_j/\lambda$)

$$\mathsf{H} \equiv \lambda \begin{pmatrix} \ddots & & & & & & \\ & -1 & (2 + v_{j-1}) & -1 & 0 & 0 & \\ & 0 & -1 & (2 + v_j) & -1 & 0 & \\ & 0 & 0 & -1 & (2 + v_{j+1}) & -1 & \\ & & & & & & \ddots \end{pmatrix} \tag{2.199}$$

and

$$\Psi \equiv \begin{pmatrix} \vdots \\ \psi_{j-1} \\ \psi_j \\ \psi_{j+1} \\ \vdots \end{pmatrix} \tag{2.200}$$

(what goes in the upper left and lower right corners of H depends on the boundary conditions, as we shall see). Evidently the allowed energies are the *eigenvalues* of the matrix H (or *would* be, in the limit $\Delta x \to 0$),[67]

Apply this method to the infinite square well. Chop the interval $(0 \le x \le a)$ into $N + 1$ equal segments (so that $\Delta x = a/(N + 1)$), letting $x_0 \equiv 0$ and $x_{N+1} \equiv a$. The boundary conditions fix $\psi_0 = \psi_{N+1} = 0$, leaving

$$\Psi \equiv \begin{pmatrix} \psi_1 \\ \vdots \\ \psi_N \end{pmatrix}. \tag{2.201}$$

[67] For further discussion see Joel Franklin, *Computational Methods for Physics* (Cambridge University Press, Cambridge, UK, 2013), Section 10.4.2.

(a) Construct the $N \times N$ matrix H, for $N = 1$, $N = 2$, and $N = 3$. (Make sure you are correctly representing Equation 2.197 for the special cases $j = 1$ and $j = N$.)

(b) Find the eigenvalues of H for these three cases "by hand," and compare them with the exact allowed energies (Equation 2.30).

(c) Using a computer (Mathematica's **Eigenvalues** package will do it) find the five lowest eigenvalues numerically for $N = 10$ and $N = 100$, and compare the exact energies.

(d) Plot (by hand) the eigen*vectors* for $N = 1, 2$, and 3, and (by computer, **Eigenvectors**) the first three eigenvectors for $N = 10$ and $N = 100$.

Solution

Begin with the Schrödinger equation.

$$i\hbar\frac{\partial \Psi}{\partial t} = -\frac{\hbar^2}{2m}\frac{\partial^2 \Psi}{\partial x^2} + V(x,t)\Psi(x,t), \quad -\infty < x < \infty,\ t > 0$$

The infinite square well potential is

$$V(x,t) = \begin{cases} 0 & \text{if } 0 \le x \le a \\ \infty & \text{else} \end{cases}.$$

Split up the PDE over the intervals where the potential is defined.

$$i\hbar\frac{\partial \Psi}{\partial t} = -\frac{\hbar^2}{2m}\frac{\partial^2 \Psi}{\partial x^2} + (\infty)\Psi(x,t), \quad x < 0,\ x > a \qquad i\hbar\frac{\partial \Psi}{\partial t} = -\frac{\hbar^2}{2m}\frac{\partial^2 \Psi}{\partial x^2}, \quad 0 \le x \le a$$

The only way to satisfy the PDE on the left is to have $\Psi(x,t) = 0$. The fact that the wave function must be continuous leads to the two Dirichlet boundary conditions, $\Psi(0,t) = 0$ and $\Psi(a,t) = 0$, for the remaining PDE.

$$\begin{aligned} & i\hbar\frac{\partial \Psi}{\partial t} = -\frac{\hbar^2}{2m}\frac{\partial^2 \Psi}{\partial x^2}, \quad 0 \le x \le a,\ t > 0 \\ & \Psi(0,t) = 0 \\ & \Psi(a,t) = 0 \end{aligned}$$

Apply the method of separation of variables since the PDE and its associated boundary conditions are linear and homogeneous: Assume a product solution for $\Psi(x,t) = \phi(t)\psi(x)$ and plug it into the PDE

$$i\hbar\frac{\partial}{\partial t}[\phi(t)\psi(x)] = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}[\phi(t)\psi(x)] \quad \rightarrow \quad i\hbar\psi(x)\frac{d\phi}{dt} = -\frac{\hbar^2}{2m}\phi(t)\frac{d^2\psi}{dx^2}$$

and the boundary conditions.

$$\begin{aligned} \Psi(0,t) &= 0 & \rightarrow \quad \phi(t)\psi(0) &= 0 & \rightarrow \quad \psi(0) &= 0 \\ \Psi(a,t) &= 0 & \rightarrow \quad \phi(t)\psi(a) &= 0 & \rightarrow \quad \psi(a) &= 0 \end{aligned}$$

Divide both sides of the PDE by $\phi(t)\psi(x)$ to separate variables.

$$i\hbar\frac{1}{\phi(t)}\frac{d\phi}{dt} = -\frac{\hbar^2}{2m}\frac{1}{\psi(x)}\frac{d^2\psi}{dx^2}$$

The only way a function of t can be equal to a function of x is if both are equal to a constant.

$$i\hbar\frac{1}{\phi(t)}\frac{d\phi}{dt} = -\frac{\hbar^2}{2m}\frac{1}{\psi(x)}\frac{d^2\psi}{dx^2} = E$$

As a result of separating variables, Schrödinger's equation has reduced to two ODEs, one in t and one in x.

$$\left.\begin{aligned} i\hbar\frac{1}{\phi(t)}\frac{d\phi}{dt} &= E \\ -\frac{\hbar^2}{2m}\frac{1}{\psi(x)}\frac{d^2\psi}{dx^2} &= E \end{aligned}\right\}$$

The ODE in x is called the time-independent Schrödinger equation (TISE).

$$\frac{d^2\psi}{dx^2} = -\frac{2mE}{\hbar^2}\psi(x), \quad \psi(0) = 0, \ \psi(a) = 0$$

Apply the finite difference method in order to solve it: Replace the second derivative with a centered second difference and discretize the $0 \le x \le a$ interval into $N+1$ equal pieces. The continuous variable x becomes a discrete one $x_j = j\Delta x$, where $j = 0, 1, \ldots, N+1$ and $\Delta x = a/(N+1)$ is the mesh size.

$$\frac{\psi_{j+1} - 2\psi_j + \psi_{j-1}}{(\Delta x)^2} = -\frac{2mE}{\hbar^2}\psi(x_j), \quad \psi(x_0) = 0, \ \psi(x_{N+1}) = 0$$

$$-\frac{\hbar^2}{2m}\left(\frac{\psi_{j+1} - 2\psi_j + \psi_{j-1}}{(\Delta x)^2}\right) = E\psi_j, \quad \psi_0 = 0, \ \psi_{N+1} = 0$$

$$\frac{\hbar^2}{2m\,(\Delta x)^2}(-\psi_{j+1} + 2\psi_j - \psi_{j-1}) = E\psi_j$$

The scheme for the unknowns is therefore

$$\boxed{\frac{(N+1)^2\hbar^2}{2ma^2}(-\psi_{j+1} + 2\psi_j - \psi_{j-1}) = E\psi_j, \quad j = 1, 2, \ldots, N.}$$

For $N = 1$,

$$\frac{2\hbar^2}{ma^2}(-\psi_2 + 2\psi_1 - \psi_0) = E\psi_1 \qquad \Rightarrow \quad \frac{2\hbar^2}{ma^2}\begin{bmatrix} 2 \end{bmatrix}\begin{bmatrix} \psi_1 \end{bmatrix} = E\begin{bmatrix} \psi_1 \end{bmatrix} \qquad \Rightarrow \quad \mathsf{H} = \frac{2\hbar^2}{ma^2}\begin{bmatrix} 2 \end{bmatrix}.$$

For $N = 2$,

$$\begin{cases} \dfrac{9\hbar^2}{2ma^2}(-\psi_2 + 2\psi_1 - \psi_0) = E\psi_1 \\ \dfrac{9\hbar^2}{2ma^2}(-\psi_3 + 2\psi_2 - \psi_1) = E\psi_2 \end{cases} \quad \Rightarrow \quad \frac{9\hbar^2}{2ma^2}\begin{bmatrix} 2 & -1 \\ -1 & 2 \end{bmatrix}\begin{bmatrix} \psi_1 \\ \psi_2 \end{bmatrix} = E\begin{bmatrix} \psi_1 \\ \psi_2 \end{bmatrix} \quad \Rightarrow \quad \mathsf{H} = \frac{9\hbar^2}{2ma^2}\begin{bmatrix} 2 & -1 \\ -1 & 2 \end{bmatrix}.$$

For $N = 3$,

$$\begin{cases} \frac{8\hbar^2}{ma^2}(-\psi_2 + 2\psi_1 - \psi_0) = E\psi_1 \\ \frac{8\hbar^2}{ma^2}(-\psi_3 + 2\psi_2 - \psi_1) = E\psi_2 \\ \frac{8\hbar^2}{ma^2}(-\psi_4 + 2\psi_3 - \psi_2) = E\psi_3 \end{cases} \quad \Rightarrow \quad \frac{8\hbar^2}{ma^2}\begin{bmatrix} 2 & -1 & 0 \\ -1 & 2 & -1 \\ 0 & -1 & 2 \end{bmatrix}\begin{bmatrix} \psi_1 \\ \psi_2 \\ \psi_3 \end{bmatrix} = E\begin{bmatrix} \psi_1 \\ \psi_2 \\ \psi_3 \end{bmatrix} \quad \Rightarrow \quad \mathsf{H} = \frac{8\hbar^2}{ma^2}\begin{bmatrix} 2 & -1 & 0 \\ -1 & 2 & -1 \\ 0 & -1 & 2 \end{bmatrix}.$$

Recognizing the pattern, the H matrix for any value of N can be constructed.

$$N = 5: \quad \mathsf{H} = \frac{18\hbar^2}{ma^2}\begin{bmatrix} 2 & -1 & 0 & 0 & 0 \\ -1 & 2 & -1 & 0 & 0 \\ 0 & -1 & 2 & -1 & 0 \\ 0 & 0 & -1 & 2 & -1 \\ 0 & 0 & 0 & -1 & 2 \end{bmatrix}$$

$$N = 10: \quad \mathsf{H} = \frac{121\hbar^2}{2ma^2}\begin{bmatrix} 2 & -1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ -1 & 2 & -1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & -1 & 2 & -1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & -1 & 2 & -1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -1 & 2 & -1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & -1 & 2 & -1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & -1 & 2 & -1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & -1 & 2 & -1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & -1 & 2 & -1 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & -1 & 2 \end{bmatrix}$$

$$N = 15: \quad \mathsf{H} = \frac{128\hbar^2}{ma^2}\begin{bmatrix} 2 & -1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ -1 & 2 & -1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & -1 & 2 & -1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & -1 & 2 & -1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -1 & 2 & -1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & -1 & 2 & -1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & -1 & 2 & -1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & -1 & 2 & -1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & -1 & 2 & -1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & -1 & 2 & -1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & -1 & 2 & -1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & -1 & 2 & -1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & -1 & 2 & -1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & -1 & 2 & -1 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & -1 & 2 \end{bmatrix}$$

The H matrix for $N = 100$ is similar but with a hundred rows and a hundred columns and $10201\hbar^2/(2ma^2)$ for the coefficient.

In any case, the scheme is an (approximate) eigenvalue problem that becomes more accurate the higher N is.

$$\mathsf{H}\Psi = E\Psi$$

Combine the two terms by using the identity matrix I.

$$(\mathsf{H} - E\mathsf{I})\Psi = \mathbf{0} \tag{1}$$

The eigenvalues satisfy

$$\det(\mathsf{H} - E\mathsf{I}) = 0.$$

For $N = 1$,

$$\left|\frac{4\hbar^2}{ma^2} - E\right| = 0 \quad \rightarrow \quad E = \frac{4\hbar^2}{ma^2}.$$

For $N = 2$,

$$\begin{vmatrix} \frac{9\hbar^2}{ma^2} - E & -\frac{9\hbar^2}{2ma^2} \\ -\frac{9\hbar^2}{2ma^2} & \frac{9\hbar^2}{ma^2} - E \end{vmatrix} = 0 \quad \rightarrow \quad \left(\frac{9\hbar^2}{ma^2} - E\right)^2 - \left(-\frac{9\hbar^2}{2ma^2}\right)^2 = 0 \quad \rightarrow \quad E = \left\{\frac{4.5\hbar^2}{ma^2}, \frac{13.5\hbar^2}{ma^2}\right\}.$$

For $N = 3$,

$$\begin{vmatrix} \frac{16\hbar^2}{ma^2} - E & -\frac{8\hbar^2}{ma^2} & 0 \\ -\frac{8\hbar^2}{ma^2} & \frac{16\hbar^2}{ma^2} - E & -\frac{8\hbar^2}{ma^2} \\ 0 & -\frac{8\hbar^2}{ma^2} & \frac{16\hbar^2}{ma^2} - E \end{vmatrix} = 0 \quad \rightarrow \quad \left(\frac{16\hbar^2}{ma^2} - E\right)\begin{vmatrix} \frac{16\hbar^2}{ma^2} - E & -\frac{8\hbar^2}{ma^2} \\ -\frac{8\hbar^2}{ma^2} & \frac{16\hbar^2}{ma^2} - E \end{vmatrix} + \frac{8\hbar^2}{ma^2}\begin{vmatrix} -\frac{8\hbar^2}{ma^2} & -\frac{8\hbar^2}{ma^2} \\ 0 & \frac{16\hbar^2}{ma^2} - E \end{vmatrix} = 0.$$

$$E = \left\{\frac{4.686291501015239\hbar^2}{ma^2}, \frac{16\hbar^2}{ma^2}, \frac{27.31370849898476\hbar^2}{ma^2}\right\}$$

Use Mathematica to find the five eigenvalues of the H matrix for $N = 5$.

$$E = \left\{\frac{4.8230854637602105\hbar^2}{ma^2}, \frac{18\hbar^2}{ma^2}, \frac{36\hbar^2}{ma^2}, \frac{54\hbar^2}{ma^2}, \frac{67.17691453623979\hbar^2}{ma^2}\right\}$$

Use Mathematica to find the lowest five eigenvalues of the H matrix for $N = 10$.

$$E = \left\{\frac{4.901350192645816\hbar^2}{ma^2}, \frac{19.20832252742708\hbar^2}{ma^2}, \frac{41.76185119262051\hbar^2}{ma^2}, \frac{70.73478342677174\hbar^2}{ma^2}, \frac{103.7799045689325\hbar^2}{ma^2}, \ldots\right\}$$

Use Mathematica to find the lowest five eigenvalues of the H matrix for $N = 15$.

$$E = \left\{\frac{4.91896821677301\hbar^2}{ma^2}, \frac{19.486839677110595\hbar^2}{ma^2}, \frac{43.14377925054842\hbar^2}{ma^2}, \frac{74.98066401624382\hbar^2}{ma^2}, \frac{113.77402034698181\hbar^2}{ma^2}, \ldots\right\}$$

Use Mathematica to find the lowest five eigenvalues of the H matrix for $N = 20$.

$$E = \left\{\frac{4.925605634718312\hbar^2}{ma^2}, \frac{19.592392648311936\hbar^2}{ma^2}, \frac{43.67272925503316\hbar^2}{ma^2}, \frac{76.62870052664626\hbar^2}{ma^2}, \frac{117.72412452304658\hbar^2}{ma^2}, \ldots\right\}$$

The exact eigenvalues of the infinite square well are known to be $n^2\pi^2\hbar^2/(2ma^2)$ with $n = 1, 2, \ldots$, the five lowest being

$$E = \left\{\frac{4.934802201926458 16\hbar^2}{ma^2}, \frac{19.73920882742708\hbar^2}{ma^2}, \frac{44.41321989262051\hbar^2}{ma^2}, \frac{78.95683521677174\hbar^2}{ma^2}, \frac{123.3700555689325\hbar^2}{ma^2}, \ldots\right\}.$$

Use the formula for percent difference,

$$\frac{\text{Approximate\_Value} - \text{Exact\_Value}}{\text{Exact\_Value}} \times 100\%,$$

and make a table that shows how good each approximation is.

	EVAL1	EVAL2	EVAL3	EVAL4	EVAL5
N=1	-18.94131%				
N=2	-8.81093%	-31.6082%			
N=3	-5.03588%	-18.9431%	-38.5009%		
N=5	-2.26385%	-8.81093%	-18.9431%	-31.6082%	-45.5484%
N=10	-0.677879%	-2.6895%	-5.96977%	-10.4134%	-15.8792%
N=15	-0.320864%	-1.27852%	-2.85825%	-5.03588%	-7.77825%
N=20	-0.186361%	-0.743779%	-1.66728%	-2.94862%	-4.57642%

Recall the following numerical integration formulas for intervals over $N+1$ pieces.

Trapezoidal Rule: $$\int_0^a f(x)\,dx \approx \frac{a}{2(N+1)}\left[f(x_0) + 2f(x_1) + 2f(x_2) + \cdots + 2f(x_N) + f(x_{N+1})\right]$$

Simpson's Rule: $$\int_0^a f(x)\,dx \approx \frac{a}{3(N+1)}\left[f(x_0) + 4f(x_1) + 2f(x_2) + 4f(x_3) + \cdots + 2f(x_{N-1}) + 4f(x_N) + f(x_{N+1})\right]$$

Simpson's rule is usually more accurate because it uses parabolas rather than trapezoids to approximate the area under the curve, but it can only be used when $N+1$ is even. Substitute each of the eigenvalues back into equation (1) to determine the corresponding eigenvectors.

For $N = 1$,

$$(\mathsf{H} - E_1\mathsf{I})\Psi_1 = \mathbf{0} \quad \rightarrow \quad \left(\frac{2\hbar^2}{ma^2}\begin{bmatrix}2\end{bmatrix} - \frac{4\hbar^2}{ma^2}\begin{bmatrix}1\end{bmatrix}\right)\begin{bmatrix}\psi_1\end{bmatrix} = \begin{bmatrix}0\end{bmatrix} \quad \rightarrow \quad \begin{bmatrix}0\end{bmatrix}\begin{bmatrix}\psi_1\end{bmatrix} = \begin{bmatrix}0\end{bmatrix}.$$

ψ_1 is arbitrary and is chosen so that the eigenvector is normalized. Use Simpson's rule.

$$1 = \int_0^a |\psi|^2\,dx \approx \frac{a}{6}\left\{[\psi(x_0)]^2 + 4[\psi(x_1)]^2 + [\psi(x_2)]^2\right\} \quad \rightarrow \quad 1 = \frac{a}{6}(4\psi_1^2) \quad \rightarrow \quad \psi_1 = \sqrt{\frac{3}{2a}}$$

Therefore, the eigenvector corresponding to

$$E_1 = \frac{4\hbar^2}{ma^2} \quad \text{is} \quad \Psi_1 = \begin{bmatrix}\sqrt{\frac{3}{2a}}\end{bmatrix}.$$

For $N = 2$,

$$(\mathsf{H} - E_1\mathsf{I})\Psi_1 = \mathbf{0} \quad \rightarrow \quad \left(\frac{9\hbar^2}{2ma^2}\begin{bmatrix}2 & -1\\-1 & 2\end{bmatrix} - \frac{4.5\hbar^2}{ma^2}\begin{bmatrix}1 & 0\\0 & 1\end{bmatrix}\right)\begin{bmatrix}\psi_1\\\psi_2\end{bmatrix} = \begin{bmatrix}0\\0\end{bmatrix} \quad \rightarrow \quad \begin{bmatrix}\frac{4.5\hbar^2}{ma^2} & -\frac{4.5\hbar^2}{ma^2}\\-\frac{4.5\hbar^2}{ma^2} & \frac{4.5\hbar^2}{ma^2}\end{bmatrix}\begin{bmatrix}\psi_1\\\psi_2\end{bmatrix} = \begin{bmatrix}0\\0\end{bmatrix}.$$

Solve the system of equations.

$$\frac{4.5\hbar^2}{ma^2}\psi_1 - \frac{4.5\hbar^2}{ma^2}\psi_2 = 0 \quad \rightarrow \quad \psi_1 = \psi_2 \quad \Rightarrow \quad \Psi_1 = \begin{bmatrix}\psi_1\\\psi_2\end{bmatrix} = \begin{bmatrix}\psi_1\\\psi_1\end{bmatrix}$$

ψ_1 is arbitrary and is chosen so that the eigenvector is normalized. Use the trapezoidal rule.

$$1 = \int_0^a |\psi|^2\,dx \approx \frac{a}{6}\left\{[\psi(x_0)]^2 + 2[\psi(x_1)]^2 + 2[\psi(x_2)]^2 + [\psi(x_3)]^2\right\} \quad \rightarrow \quad 1 = \frac{a}{6}(4\psi_1^2) \quad \rightarrow \quad \psi_1 = \sqrt{\frac{3}{2a}}$$

Therefore, the eigenvector corresponding to

$$E_1 = \frac{4.5\hbar^2}{ma^2} \quad \text{is} \quad \Psi_1 = \begin{bmatrix} \sqrt{\frac{3}{2a}} \\ \sqrt{\frac{3}{2a}} \end{bmatrix}.$$

For $N = 2$ also,

$$(\mathsf{H} - E_2\mathsf{I})\Psi_2 = \mathbf{0} \quad \rightarrow \quad \left(\frac{9\hbar^2}{2ma^2}\begin{bmatrix} 2 & -1 \\ -1 & 2 \end{bmatrix} - \frac{13.5\hbar^2}{ma^2}\begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}\right)\begin{bmatrix} \psi_1 \\ \psi_2 \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \end{bmatrix} \quad \rightarrow \quad \begin{bmatrix} -\frac{4.5\hbar^2}{ma^2} & -\frac{4.5\hbar^2}{ma^2} \\ -\frac{4.5\hbar^2}{ma^2} & -\frac{4.5\hbar^2}{ma^2} \end{bmatrix}\begin{bmatrix} \psi_1 \\ \psi_2 \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \end{bmatrix}.$$

Solve the system of equations.

$$-\frac{4.5\hbar^2}{ma^2}\psi_1 - \frac{4.5\hbar^2}{ma^2}\psi_2 = 0 \quad \rightarrow \quad \psi_2 = -\psi_1 \quad \Rightarrow \quad \Psi_2 = \begin{bmatrix} \psi_1 \\ \psi_2 \end{bmatrix} = \begin{bmatrix} \psi_1 \\ -\psi_1 \end{bmatrix}$$

ψ_1 is arbitrary and is chosen so that the eigenvector is normalized. Use the trapezoidal rule.

$$1 = \int_0^a |\psi|^2\,dx \approx \frac{a}{6}\left\{[\psi(x_0)]^2 + 2[\psi(x_1)]^2 + 2[\psi(x_2)]^2 + [\psi(x_3)]^2\right\} \quad \rightarrow \quad 1 = \frac{a}{6}(4\psi_1^2) \quad \rightarrow \quad \psi_1 = \sqrt{\frac{3}{2a}}$$

Therefore, the eigenvector corresponding to

$$E_2 = \frac{13.5\hbar^2}{ma^2} \quad \text{is} \quad \Psi_2 = \begin{bmatrix} \sqrt{\frac{3}{2a}} \\ -\sqrt{\frac{3}{2a}} \end{bmatrix}.$$

For $N = 3$,

$$(\mathsf{H} - E_1\mathsf{I})\Psi_1 = \mathbf{0} \quad \rightarrow \quad \left(\frac{8\hbar^2}{ma^2}\begin{bmatrix} 2 & -1 & 0 \\ -1 & 2 & -1 \\ 0 & -1 & 2 \end{bmatrix} - \frac{8(2-\sqrt{2})\hbar^2}{ma^2}\begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}\right)\begin{bmatrix} \psi_1 \\ \psi_2 \\ \psi_3 \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ 0 \end{bmatrix}$$

$$\begin{bmatrix} \frac{8\sqrt{2}\hbar^2}{ma^2} & -\frac{8\hbar^2}{ma^2} & 0 \\ -\frac{8\hbar^2}{ma^2} & \frac{8\sqrt{2}\hbar^2}{ma^2} & -\frac{8\hbar^2}{ma^2} \\ 0 & -\frac{8\hbar^2}{ma^2} & \frac{8\sqrt{2}\hbar^2}{ma^2} \end{bmatrix}\begin{bmatrix} \psi_1 \\ \psi_2 \\ \psi_3 \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ 0 \end{bmatrix}.$$

Solve the system of equations.

$$\begin{cases} \frac{8\sqrt{2}\hbar^2}{ma^2}\psi_1 - \frac{8\hbar^2}{ma^2}\psi_2 = 0 \\ -\frac{8\hbar^2}{ma^2}\psi_2 + \frac{8\sqrt{2}\hbar^2}{ma^2}\psi_3 = 0 \end{cases} \quad \rightarrow \quad \begin{cases} \psi_1 = \frac{1}{\sqrt{2}}\psi_2 \\ \psi_3 = \frac{1}{\sqrt{2}}\psi_2 \end{cases} \quad \Rightarrow \quad \Psi_1 = \begin{bmatrix} \psi_1 \\ \psi_2 \\ \psi_3 \end{bmatrix} = \begin{bmatrix} \frac{1}{\sqrt{2}}\psi_2 \\ \psi_2 \\ \frac{1}{\sqrt{2}}\psi_2 \end{bmatrix}$$

ψ_2 is arbitrary and is chosen so that the eigenvector is normalized. Use Simpson's rule.

$$1 = \int_0^a |\psi|^2\,dx \approx \frac{a}{12}\left\{[\psi(x_0)]^2 + 4[\psi(x_1)]^2 + 2[\psi(x_2)]^2 + 4[\psi(x_3)]^2 + [\psi(x_4)]^2\right\}$$

$$1 = \frac{a}{12}\left[4\left(\frac{1}{2}\psi_2^2\right) + 2\psi_2^2 + 4\left(\frac{1}{2}\psi_2^2\right)\right]$$

$$\psi_2 = \sqrt{\frac{2}{a}}$$

Therefore, the eigenvector corresponding to

$$E_1 = \frac{8(2-\sqrt{2})\hbar^2}{ma^2} \quad \text{is} \quad \Psi_1 = \begin{bmatrix} \frac{1}{\sqrt{a}} \\ \sqrt{\frac{2}{a}} \\ \frac{1}{\sqrt{a}} \end{bmatrix}.$$

For $N = 3$ also,

$$(\mathsf{H} - E_2\mathsf{I})\Psi_2 = \mathbf{0} \quad \rightarrow \quad \left(\frac{8\hbar^2}{ma^2}\begin{bmatrix} 2 & -1 & 0 \\ -1 & 2 & -1 \\ 0 & -1 & 2 \end{bmatrix} - \frac{16\hbar^2}{ma^2}\begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}\right)\begin{bmatrix} \psi_1 \\ \psi_2 \\ \psi_3 \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ 0 \end{bmatrix}$$

$$\begin{bmatrix} 0 & -\frac{8\hbar^2}{ma^2} & 0 \\ -\frac{8\hbar^2}{ma^2} & 0 & -\frac{8\hbar^2}{ma^2} \\ 0 & -\frac{8\hbar^2}{ma^2} & 0 \end{bmatrix}\begin{bmatrix} \psi_1 \\ \psi_2 \\ \psi_3 \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ 0 \end{bmatrix}.$$

Solve the system of equations.

$$\begin{cases} -\dfrac{8\hbar^2}{ma^2}\psi_2 = 0 \\ -\dfrac{8\hbar^2}{ma^2}\psi_1 - \dfrac{8\hbar^2}{ma^2}\psi_3 = 0 \end{cases} \quad \rightarrow \quad \begin{cases} \psi_2 = 0 \\ \psi_3 = -\psi_1 \end{cases} \quad \Rightarrow \quad \Psi_2 = \begin{bmatrix} \psi_1 \\ \psi_2 \\ \psi_3 \end{bmatrix} = \begin{bmatrix} \psi_1 \\ 0 \\ -\psi_1 \end{bmatrix}$$

ψ_1 is arbitrary and is chosen so that the eigenvector is normalized. Use Simpson's rule.

$$1 = \int_0^a |\psi|^2\,dx \approx \frac{a}{12}\left\{[\psi(x_0)]^2 + 4[\psi(x_1)]^2 + 2[\psi(x_2)]^2 + 4[\psi(x_3)]^2 + [\psi(x_4)]^2\right\}$$

$$1 = \frac{a}{12}\left(4\psi_1^2 + 4\psi_1^2\right)$$

$$\psi_1 = \sqrt{\frac{3}{2a}}$$

Therefore, the eigenvector corresponding to

$$E_2 = \frac{16\hbar^2}{ma^2} \quad \text{is} \quad \Psi_2 = \begin{bmatrix} \sqrt{\frac{3}{2a}} \\ 0 \\ -\sqrt{\frac{3}{2a}} \end{bmatrix}.$$

For $N = 3$ also,

$$(\mathsf{H} - E_3\mathsf{I})\Psi_3 = \mathbf{0} \quad \rightarrow \quad \left(\frac{8\hbar^2}{ma^2}\begin{bmatrix} 2 & -1 & 0 \\ -1 & 2 & -1 \\ 0 & -1 & 2 \end{bmatrix} - \frac{8(2+\sqrt{2})\hbar^2}{ma^2}\begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}\right)\begin{bmatrix} \psi_1 \\ \psi_2 \\ \psi_3 \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ 0 \end{bmatrix}$$

$$\begin{bmatrix} -\frac{8\sqrt{2}\hbar^2}{ma^2} & -\frac{8\hbar^2}{ma^2} & 0 \\ -\frac{8\hbar^2}{ma^2} & -\frac{8\sqrt{2}\hbar^2}{ma^2} & -\frac{8\hbar^2}{ma^2} \\ 0 & -\frac{8\hbar^2}{ma^2} & -\frac{8\sqrt{2}\hbar^2}{ma^2} \end{bmatrix}\begin{bmatrix} \psi_1 \\ \psi_2 \\ \psi_3 \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ 0 \end{bmatrix}.$$

Solve the system of equations.

$$\begin{cases} -\dfrac{8\sqrt{2}\hbar^2}{ma^2}\psi_1 - \dfrac{8\hbar^2}{ma^2}\psi_2 = 0 \\ -\dfrac{8\hbar^2}{ma^2}\psi_2 - \dfrac{8\sqrt{2}\hbar^2}{ma^2}\psi_3 = 0 \end{cases} \quad \rightarrow \quad \begin{cases} \psi_1 = -\dfrac{1}{\sqrt{2}}\psi_2 \\ \psi_3 = -\dfrac{1}{\sqrt{2}}\psi_2 \end{cases} \quad \Rightarrow \quad \Psi_3 = \begin{bmatrix} \psi_1 \\ \psi_2 \\ \psi_3 \end{bmatrix} = \begin{bmatrix} -\frac{1}{\sqrt{2}}\psi_2 \\ \psi_2 \\ -\frac{1}{\sqrt{2}}\psi_2 \end{bmatrix}$$

ψ_2 is arbitrary and is chosen so that the eigenvector is normalized. Use Simpson's rule.

$$1 = \int_0^a |\psi|^2\,dx \approx \frac{a}{12}\left\{[\psi(x_0)]^2 + 4[\psi(x_1)]^2 + 2[\psi(x_2)]^2 + 4[\psi(x_3)]^2 + [\psi(x_4)]^2\right\}$$

$$1 = \frac{a}{12}\left[4\left(\frac{1}{2}\psi_2^2\right) + 2\psi_2^2 + 4\left(\frac{1}{2}\psi_2^2\right)\right]$$

$$\psi_2 = -\sqrt{\frac{2}{a}}$$

Therefore, the eigenvector corresponding to

$$E_3 = \frac{8(2+\sqrt{2})\hbar^2}{ma^2} \quad \text{is} \quad \Psi_3 = \begin{bmatrix} \frac{1}{\sqrt{a}} \\ -\sqrt{\frac{2}{a}} \\ \frac{1}{\sqrt{a}} \end{bmatrix}.$$

Use Mathematica to find the five eigenvectors (corresponding to the eigenvalues in the same order) of the H matrix for $N = 5$. Normalize them as well using Simpson's rule.

$$\Psi_1 = \begin{bmatrix} \frac{1}{\sqrt{2a}} \\ \sqrt{\frac{3}{2a}} \\ \sqrt{\frac{2}{a}} \\ \sqrt{\frac{3}{2a}} \\ \frac{1}{\sqrt{2a}} \end{bmatrix} \quad \Psi_2 = \begin{bmatrix} \sqrt{\frac{3}{2a}} \\ \sqrt{\frac{3}{2a}} \\ 0 \\ -\sqrt{\frac{3}{2a}} \\ -\sqrt{\frac{3}{2a}} \end{bmatrix} \quad \Psi_3 = \begin{bmatrix} \sqrt{\frac{3}{2a}} \\ 0 \\ -\sqrt{\frac{3}{2a}} \\ 0 \\ \sqrt{\frac{3}{2a}} \end{bmatrix} \quad \Psi_4 = \begin{bmatrix} \sqrt{\frac{3}{2a}} \\ -\sqrt{\frac{3}{2a}} \\ 0 \\ \sqrt{\frac{3}{2a}} \\ -\sqrt{\frac{3}{2a}} \end{bmatrix} \quad \Psi_5 = \begin{bmatrix} \frac{1}{\sqrt{2a}} \\ -\sqrt{\frac{3}{2a}} \\ \sqrt{\frac{2}{a}} \\ -\sqrt{\frac{3}{2a}} \\ \frac{1}{\sqrt{2a}} \end{bmatrix}$$

Use Mathematica to find the five eigenvectors (corresponding to the lowest five eigenvalues in the same order) of the H matrix for $N = 10$. Normalize them as well using the trapezoidal rule.

$$\Psi_1 = \frac{1}{\sqrt{a}}\begin{bmatrix} 0.39843 \\ 0.764582 \\ 1.06879 \\ 1.28641 \\ 1.39982 \\ 1.39982 \\ 1.28641 \\ 1.06879 \\ 0.764582 \\ 0.39843 \end{bmatrix} \quad \Psi_2 = \frac{1}{\sqrt{a}}\begin{bmatrix} 0.764582 \\ 1.28641 \\ 1.39982 \\ 1.06879 \\ 0.39843 \\ -0.39843 \\ -1.06879 \\ -1.39982 \\ -1.28641 \\ -0.764582 \end{bmatrix} \quad \Psi_3 = \frac{1}{\sqrt{a}}\begin{bmatrix} 1.06879 \\ 1.39982 \\ 0.764582 \\ -0.39843 \\ -1.28641 \\ -1.28641 \\ -0.39843 \\ 0.764582 \\ 1.39982 \\ 1.06879 \end{bmatrix} \quad \Psi_4 = \frac{1}{\sqrt{a}}\begin{bmatrix} 1.28641 \\ 1.06879 \\ -0.39843 \\ -1.39982 \\ -0.764582 \\ 0.764582 \\ 1.39982 \\ 0.39843 \\ -1.06879 \\ -1.28641 \end{bmatrix} \quad \Psi_5 = \frac{1}{\sqrt{a}}\begin{bmatrix} 1.39982 \\ 0.39843 \\ -1.28641 \\ -0.764582 \\ 1.06879 \\ 1.06879 \\ -0.764582 \\ -1.28641 \\ 0.39843 \\ 1.39982 \end{bmatrix}$$

Use Mathematica to find the five eigenvectors (corresponding to the lowest five eigenvalues in the same order) of the H matrix for $N = 20$. Normalize them as well using the trapezoidal rule.

$$\Psi_1 = \begin{bmatrix} \frac{0.210778}{\sqrt{a}} \\ \frac{0.416847}{\sqrt{a}} \\ \frac{0.613604}{\sqrt{a}} \\ \frac{0.796655}{\sqrt{a}} \\ \frac{0.96191}{\sqrt{a}} \\ \frac{1.10568}{\sqrt{a}} \\ \frac{1.22474}{\sqrt{a}} \\ \frac{1.31645}{\sqrt{a}} \\ \frac{1.37876}{\sqrt{a}} \\ \frac{1.41026}{\sqrt{a}} \\ \frac{1.41026}{\sqrt{a}} \\ \frac{1.37876}{\sqrt{a}} \\ \frac{1.31645}{\sqrt{a}} \\ \frac{1.22474}{\sqrt{a}} \\ \frac{1.10568}{\sqrt{a}} \\ \frac{0.96191}{\sqrt{a}} \\ \frac{0.796655}{\sqrt{a}} \\ \frac{0.613604}{\sqrt{a}} \\ \frac{0.416847}{\sqrt{a}} \\ \frac{0.210778}{\sqrt{a}} \end{bmatrix} \quad \Psi_2 = \begin{bmatrix} \frac{0.416847}{\sqrt{a}} \\ \frac{0.796655}{\sqrt{a}} \\ \frac{1.10568}{\sqrt{a}} \\ \frac{1.31645}{\sqrt{a}} \\ \frac{1.41026}{\sqrt{a}} \\ \frac{1.37876}{\sqrt{a}} \\ \frac{1.22474}{\sqrt{a}} \\ \frac{0.96191}{\sqrt{a}} \\ \frac{0.613604}{\sqrt{a}} \\ \frac{0.210778}{\sqrt{a}} \\ -\frac{0.210778}{\sqrt{a}} \\ -\frac{0.613604}{\sqrt{a}} \\ -\frac{0.96191}{\sqrt{a}} \\ -\frac{1.22474}{\sqrt{a}} \\ -\frac{1.37876}{\sqrt{a}} \\ -\frac{1.41026}{\sqrt{a}} \\ -\frac{1.31645}{\sqrt{a}} \\ -\frac{1.10568}{\sqrt{a}} \\ -\frac{0.796655}{\sqrt{a}} \\ -\frac{0.416847}{\sqrt{a}} \end{bmatrix} \quad \Psi_3 = \begin{bmatrix} \frac{0.613604}{\sqrt{a}} \\ \frac{1.10568}{\sqrt{a}} \\ \frac{1.37876}{\sqrt{a}} \\ \frac{1.37876}{\sqrt{a}} \\ \frac{1.10568}{\sqrt{a}} \\ \frac{0.613604}{\sqrt{a}} \\ 0 \\ -\frac{0.613604}{\sqrt{a}} \\ -\frac{1.10568}{\sqrt{a}} \\ -\frac{1.37876}{\sqrt{a}} \\ -\frac{1.37876}{\sqrt{a}} \\ -\frac{1.10568}{\sqrt{a}} \\ -\frac{0.613604}{\sqrt{a}} \\ 0 \\ \frac{0.613604}{\sqrt{a}} \\ \frac{1.10568}{\sqrt{a}} \\ \frac{1.37876}{\sqrt{a}} \\ \frac{1.37876}{\sqrt{a}} \\ \frac{1.10568}{\sqrt{a}} \\ \frac{0.613604}{\sqrt{a}} \end{bmatrix} \quad \Psi_4 = \begin{bmatrix} \frac{0.796655}{\sqrt{a}} \\ \frac{1.31645}{\sqrt{a}} \\ \frac{1.37876}{\sqrt{a}} \\ \frac{0.96191}{\sqrt{a}} \\ \frac{0.210778}{\sqrt{a}} \\ -\frac{0.613604}{\sqrt{a}} \\ -\frac{1.22474}{\sqrt{a}} \\ -\frac{1.41026}{\sqrt{a}} \\ -\frac{1.10568}{\sqrt{a}} \\ -\frac{0.416847}{\sqrt{a}} \\ \frac{0.416847}{\sqrt{a}} \\ \frac{1.10568}{\sqrt{a}} \\ \frac{1.41026}{\sqrt{a}} \\ \frac{1.22474}{\sqrt{a}} \\ \frac{0.613604}{\sqrt{a}} \\ -\frac{0.210778}{\sqrt{a}} \\ -\frac{0.96191}{\sqrt{a}} \\ -\frac{1.37876}{\sqrt{a}} \\ -\frac{1.31645}{\sqrt{a}} \\ -\frac{0.796655}{\sqrt{a}} \end{bmatrix} \quad \Psi_5 = \begin{bmatrix} \frac{0.96191}{\sqrt{a}} \\ \frac{1.41026}{\sqrt{a}} \\ \frac{1.10568}{\sqrt{a}} \\ \frac{0.210778}{\sqrt{a}} \\ -\frac{0.796655}{\sqrt{a}} \\ -\frac{1.37876}{\sqrt{a}} \\ -\frac{1.22474}{\sqrt{a}} \\ -\frac{0.416847}{\sqrt{a}} \\ \frac{0.613604}{\sqrt{a}} \\ \frac{1.31645}{\sqrt{a}} \\ \frac{1.31645}{\sqrt{a}} \\ \frac{0.613604}{\sqrt{a}} \\ -\frac{0.416847}{\sqrt{a}} \\ -\frac{1.22474}{\sqrt{a}} \\ -\frac{1.37876}{\sqrt{a}} \\ -\frac{0.796655}{\sqrt{a}} \\ \frac{0.210778}{\sqrt{a}} \\ \frac{1.10568}{\sqrt{a}} \\ \frac{1.41026}{\sqrt{a}} \\ \frac{0.96191}{\sqrt{a}} \end{bmatrix}$$

The exact eigenstates of the infinite square well are known to be

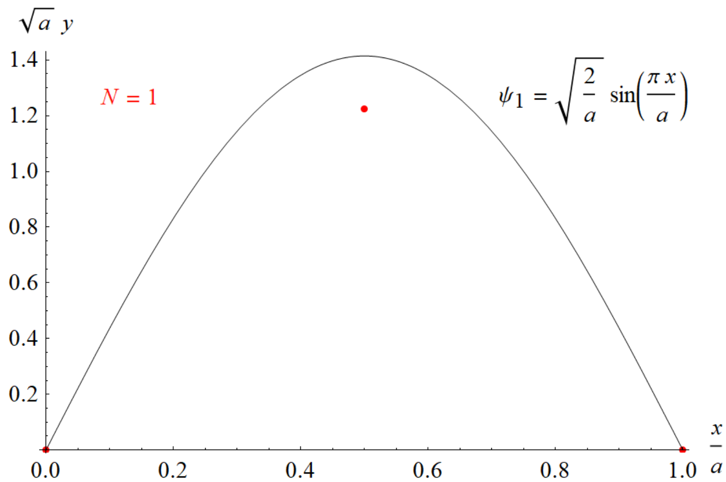
$$\psi_n(x) = \sqrt{\frac{2}{a}} \sin \frac{n\pi x}{a}, \quad n = 1, 2, \ldots,$$

the first one being

$$\psi_1(x) = \sqrt{\frac{2}{a}} \sin \frac{\pi x}{a}.$$

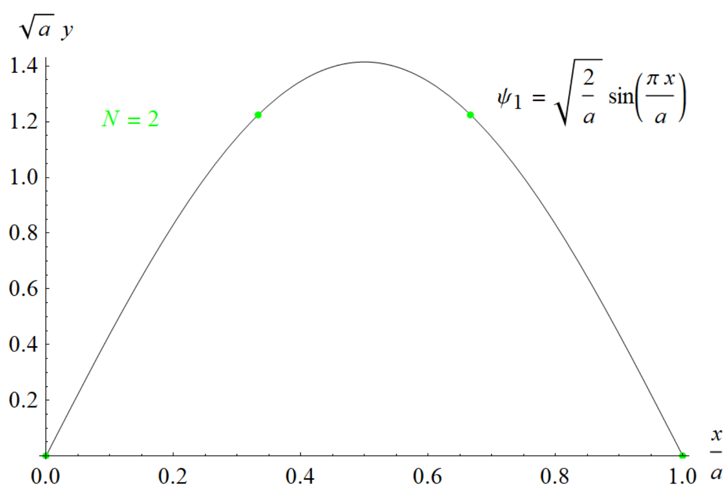
Plot it together with the $N = 1$ approximation, that is, the three points,

$$\Psi_1 = \left[\sqrt{\tfrac{3}{2a}}\right] : \qquad \left\{(0,0), \left(\frac{a}{2}, \sqrt{\frac{3}{2a}}\right), (a, 0)\right\}.$$



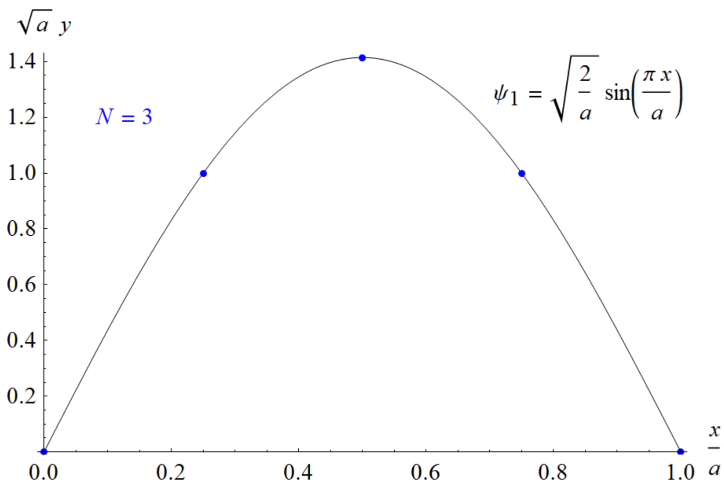
Plot the first eigenstate with the $N = 2$ approximation, that is, the four points,

$$\Psi_1 = \begin{bmatrix} \sqrt{\tfrac{3}{2a}} \\ \sqrt{\tfrac{3}{2a}} \end{bmatrix} : \qquad \left\{(0,0), \left(\frac{a}{3}, \sqrt{\frac{3}{2a}}\right), \left(\frac{2a}{3}, \sqrt{\frac{3}{2a}}\right), (a, 0)\right\}.$$



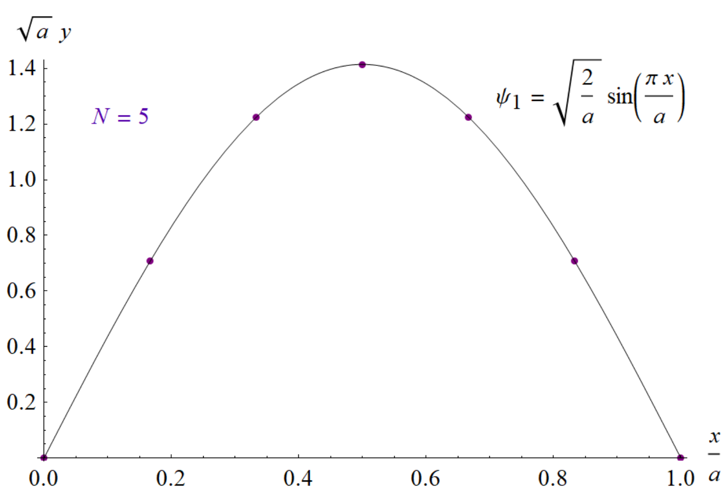
Plot the first eigenstate with the $N = 3$ approximation, that is, the five points,

$$\Psi_1 = \begin{bmatrix} \frac{1}{\sqrt{a}} \\ \sqrt{\frac{2}{a}} \\ \frac{1}{\sqrt{a}} \end{bmatrix} : \qquad \left\{(0,0), \left(\frac{a}{4}, \frac{1}{\sqrt{a}}\right), \left(\frac{a}{2}, \sqrt{\frac{2}{a}}\right), \left(\frac{3a}{4}, \frac{1}{\sqrt{a}}\right), (a,0)\right\}.$$

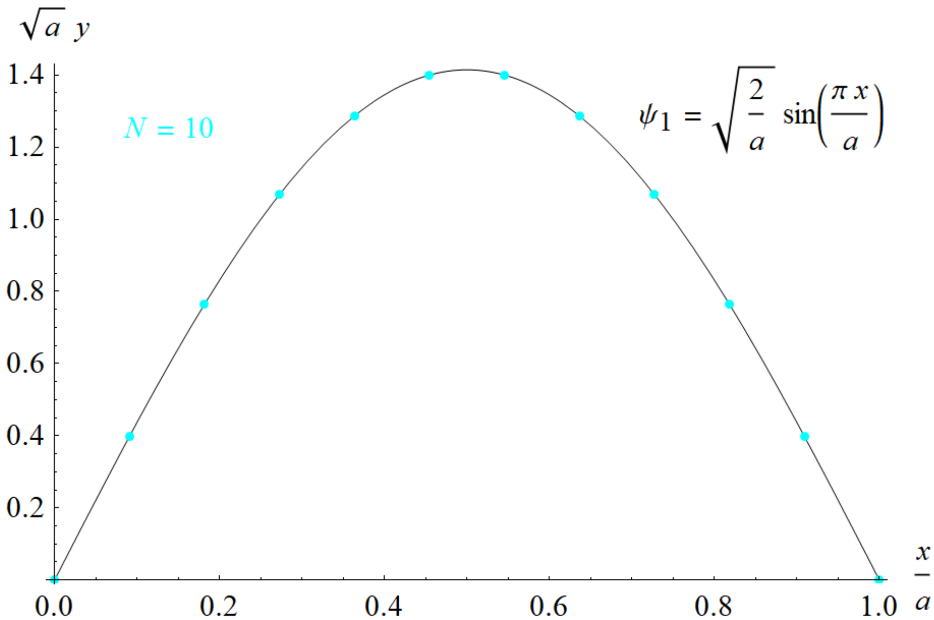


Plot the first eigenstate with the $N = 5$ approximation, that is, the seven points,

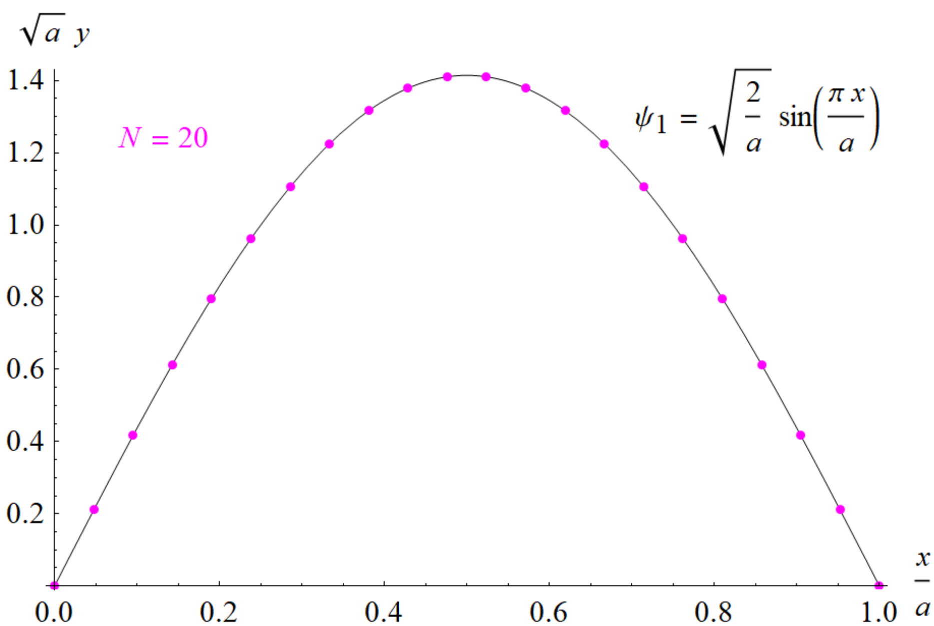
$$\Psi_1 = \begin{bmatrix} \frac{1}{\sqrt{2a}} \\ \sqrt{\frac{3}{2a}} \\ \sqrt{\frac{2}{a}} \\ \sqrt{\frac{3}{2a}} \\ \frac{1}{\sqrt{2a}} \end{bmatrix} : \qquad \left\{(0,0), \left(\frac{a}{6}, \frac{1}{\sqrt{2a}}\right), \left(\frac{a}{3}, \sqrt{\frac{3}{2a}}\right), \left(\frac{a}{2}, \sqrt{\frac{2}{a}}\right), \left(\frac{2a}{3}, \sqrt{\frac{3}{2a}}\right), \left(\frac{5a}{6}, \frac{1}{\sqrt{2a}}\right), (a,0)\right\}.$$



Plot the first eigenstate with the $N = 10$ approximation.



Plot the first eigenstate with the $N = 20$ approximation.

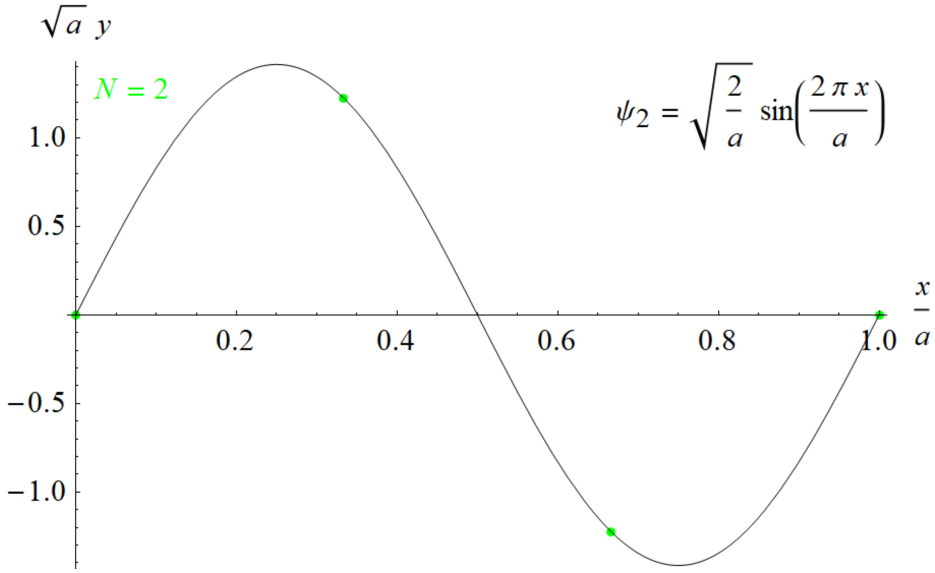


The second eigenstate is

$$\psi_2(x) = \sqrt{\frac{2}{a}} \sin \frac{2\pi x}{a}.$$

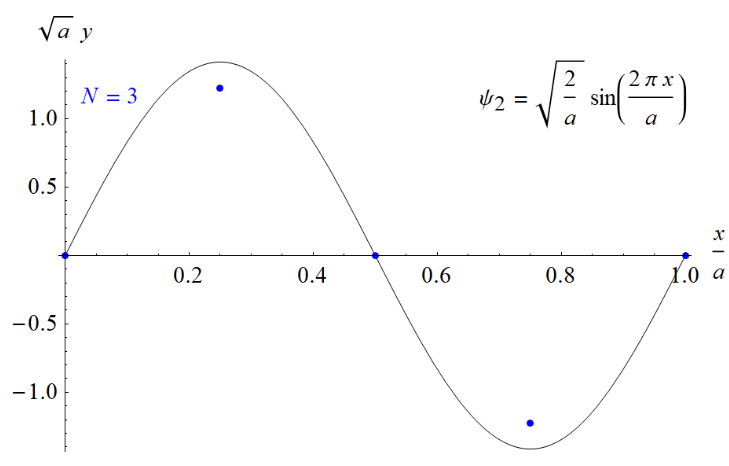
Plot it together with the $N = 2$ approximation, that is, the four points,

$$\Psi_2 = \begin{bmatrix} \sqrt{\frac{3}{2a}} \\ -\sqrt{\frac{3}{2a}} \end{bmatrix} : \qquad \left\{(0,0), \left(\frac{a}{3}, \sqrt{\frac{3}{2a}}\right), \left(\frac{2a}{3}, -\sqrt{\frac{3}{2a}}\right), (a,0)\right\}.$$



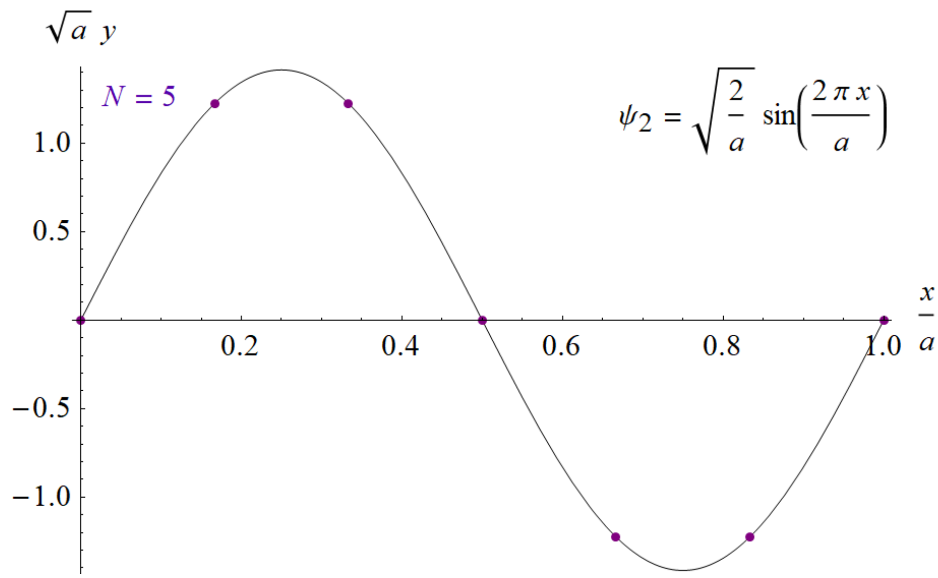
Plot the second eigenstate with the $N = 3$ approximation, that is, the five points,

$$\Psi_2 = \begin{bmatrix} \sqrt{\frac{3}{2a}} \\ 0 \\ -\sqrt{\frac{3}{2a}} \end{bmatrix} : \qquad \left\{(0,0), \left(\frac{a}{4}, \sqrt{\frac{3}{2a}}\right), \left(\frac{a}{2}, 0\right), \left(\frac{3a}{4}, -\sqrt{\frac{3}{2a}}\right), (a,0)\right\}.$$

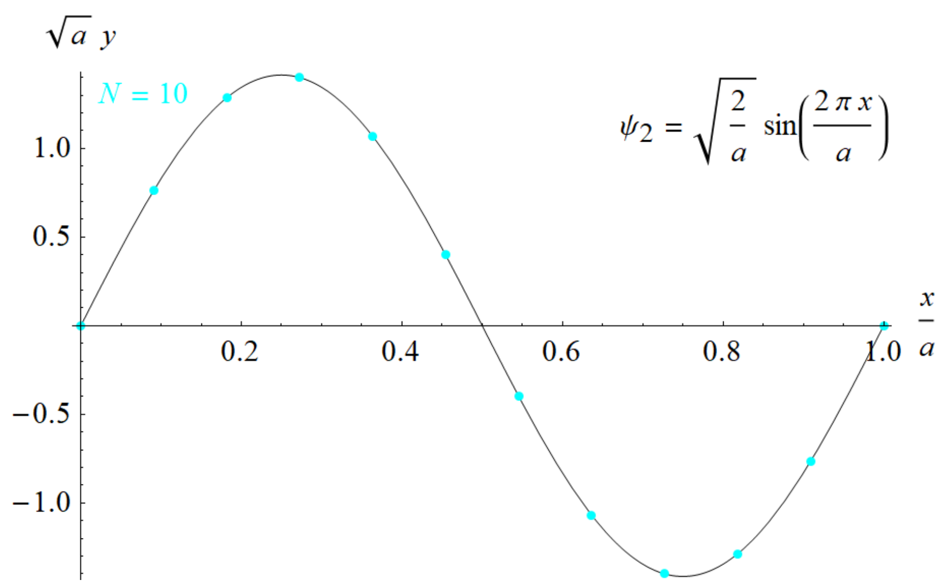


Plot the second eigenstate with the $N = 5$ approximation, that is, the seven points,

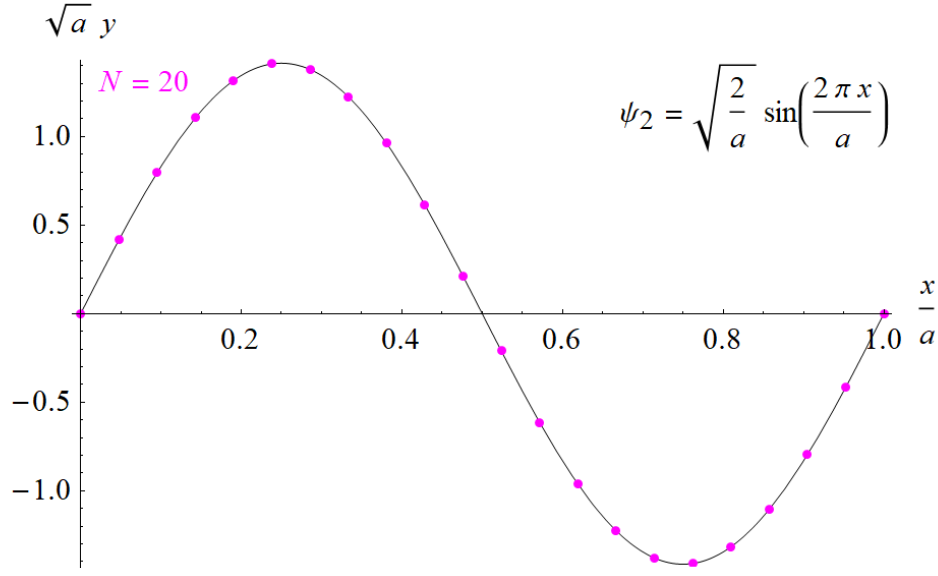
$$\Psi_2 = \begin{bmatrix} \sqrt{\frac{3}{2a}} \\ \sqrt{\frac{3}{2a}} \\ 0 \\ -\sqrt{\frac{3}{2a}} \\ -\sqrt{\frac{3}{2a}} \end{bmatrix} : \qquad \left\{(0,0), \left(\frac{a}{6}, \sqrt{\frac{3}{2a}}\right), \left(\frac{a}{3}, \sqrt{\frac{3}{2a}}\right), \left(\frac{a}{2}, 0\right), \left(\frac{2a}{3}, -\sqrt{\frac{3}{2a}}\right), \left(\frac{5a}{6}, -\sqrt{\frac{3}{2a}}\right), (a,0)\right\}.$$



Plot the second eigenstate with the $N = 10$ approximation.



Plot the second eigenstate with the $N = 20$ approximation.

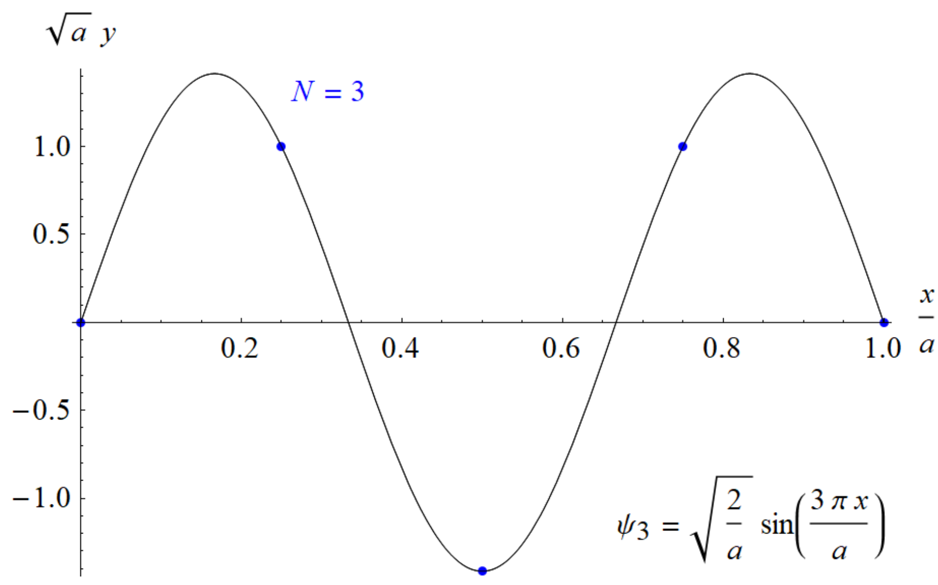


The third eigenstate is

$$\psi_3(x) = \sqrt{\frac{2}{a}} \sin \frac{3\pi x}{a}.$$

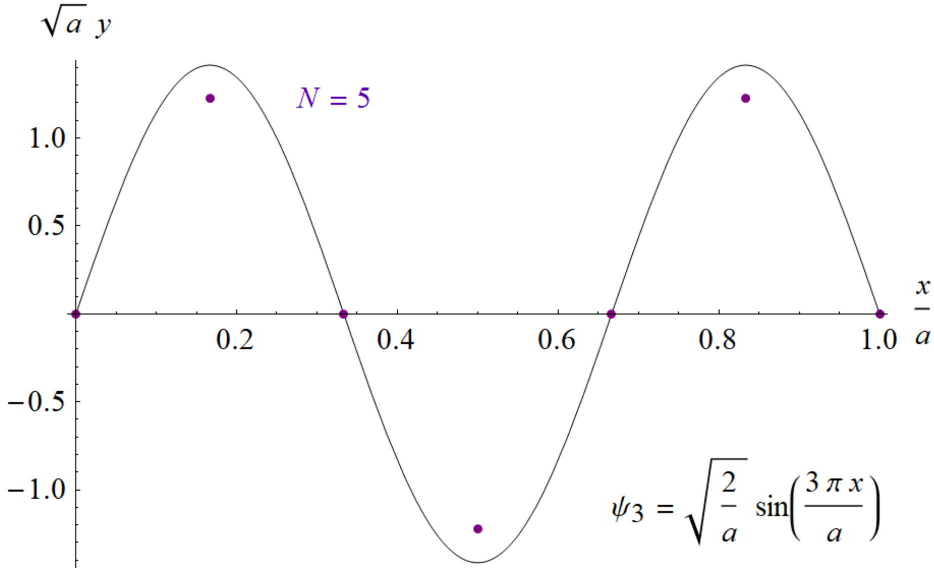
Plot it together with the $N = 3$ approximation, that is, the five points,

$$\Psi_3 = \begin{bmatrix} \frac{1}{\sqrt{a}} \\ -\sqrt{\frac{2}{a}} \\ \frac{1}{\sqrt{a}} \end{bmatrix} : \qquad \left\{ (0,0), \left(\frac{a}{4}, \frac{1}{\sqrt{a}}\right), \left(\frac{a}{2}, -\sqrt{\frac{2}{a}}\right), \left(\frac{3a}{4}, \frac{1}{\sqrt{a}}\right), (a,0) \right\}.$$

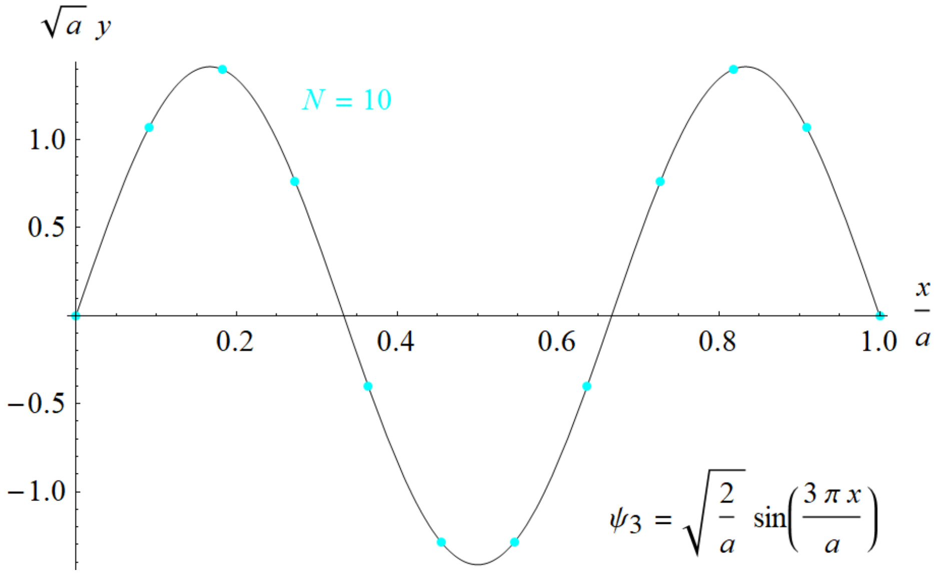


Plot the third eigenstate with the $N = 5$ approximation, that is, the seven points,

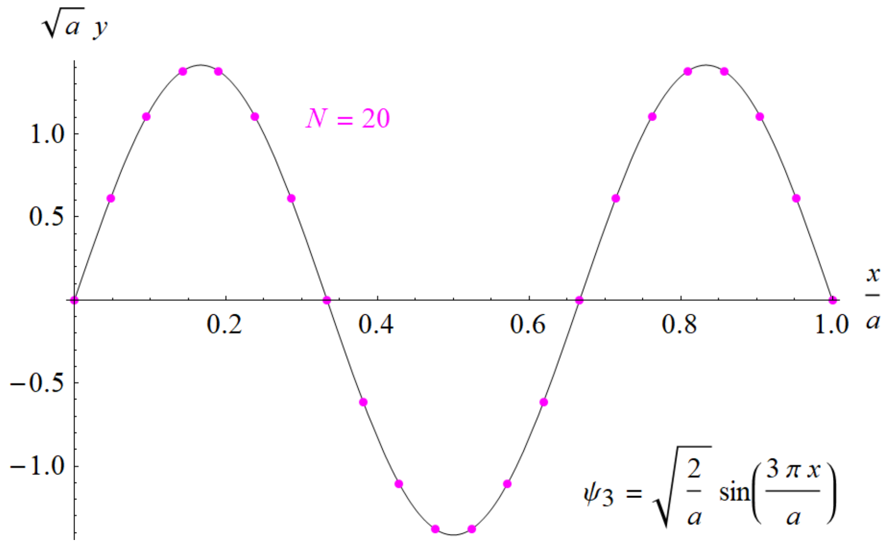
$$\Psi_3 = \begin{bmatrix} \sqrt{\frac{3}{2a}} \\ 0 \\ -\sqrt{\frac{3}{2a}} \\ 0 \\ \sqrt{\frac{3}{2a}} \end{bmatrix} : \qquad \left\{(0,0), \left(\frac{a}{6}, \sqrt{\frac{3}{2a}}\right), \left(\frac{a}{3}, 0\right), \left(\frac{a}{2}, -\sqrt{\frac{3}{2a}}\right), \left(\frac{2a}{3}, 0\right), \left(\frac{5a}{6}, \sqrt{\frac{3}{2a}}\right), (a,0)\right\}.$$



Plot the third eigenstate with the $N = 10$ approximation.



Plot the third eigenstate with the $N = 20$ approximation.

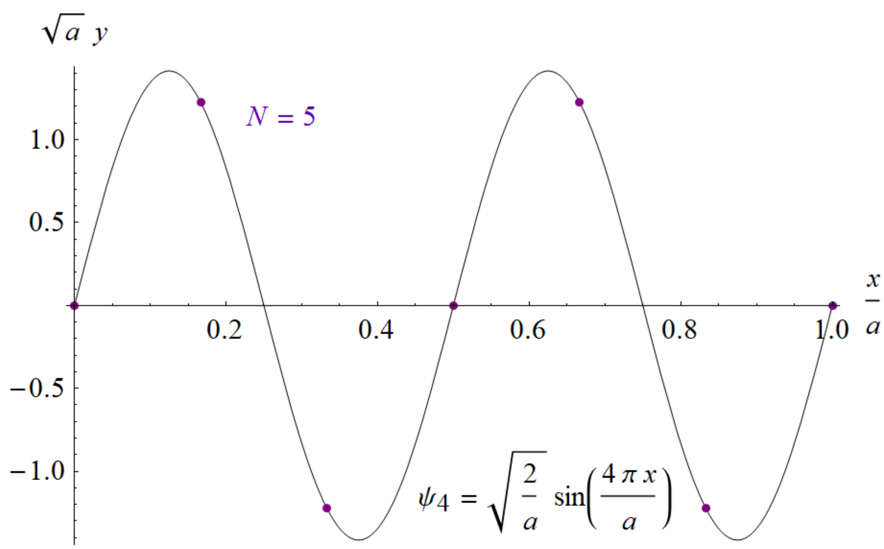


The fourth eigenstate is

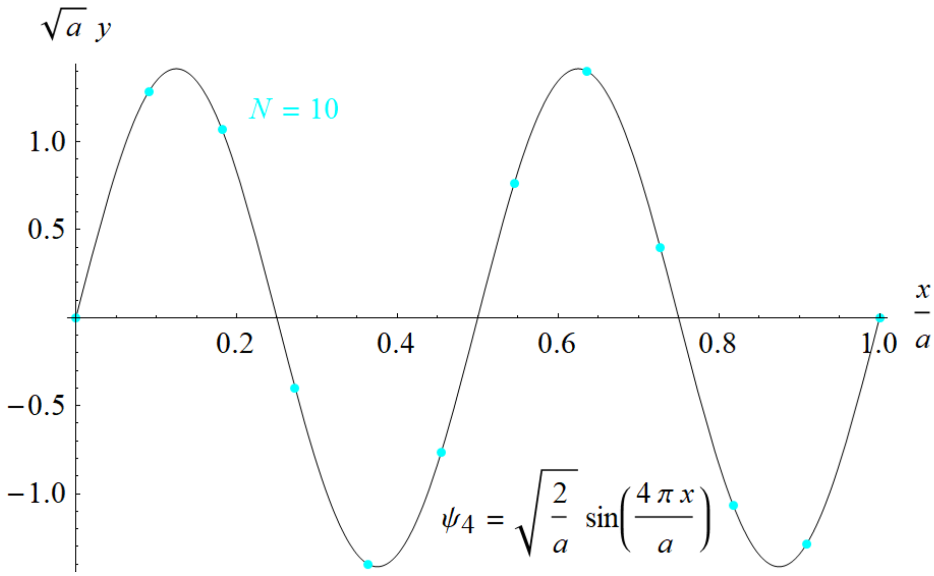
$$\psi_4(x) = \sqrt{\frac{2}{a}} \sin \frac{4\pi x}{a}.$$

Plot it together with the $N = 5$ approximation, that is, the seven points,

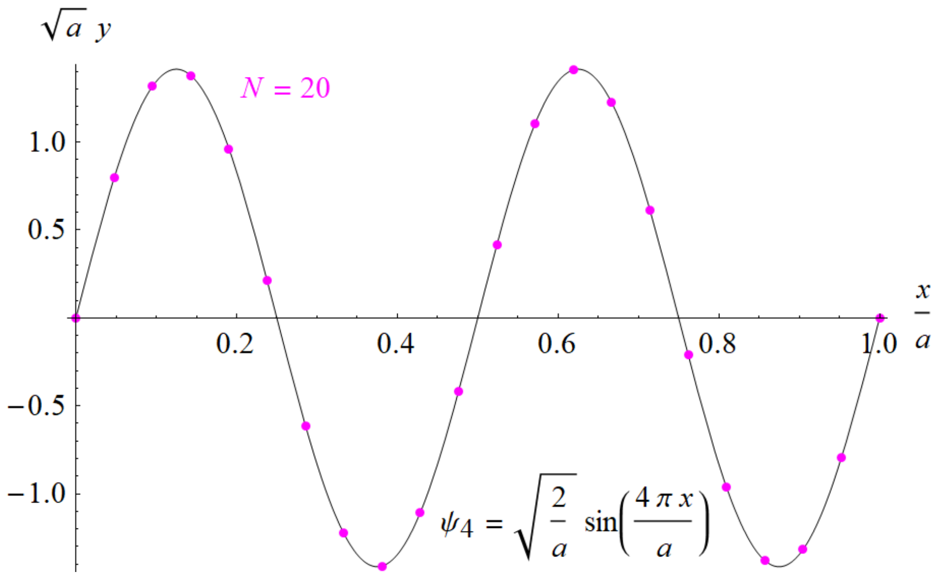
$$\Psi_4 = \begin{bmatrix} \sqrt{\frac{3}{2a}} \\ -\sqrt{\frac{3}{2a}} \\ 0 \\ \sqrt{\frac{3}{2a}} \\ -\sqrt{\frac{3}{2a}} \end{bmatrix} : \qquad \left\{(0,0), \left(\frac{a}{6}, \sqrt{\frac{3}{2a}}\right), \left(\frac{a}{3}, -\sqrt{\frac{3}{2a}}\right), \left(\frac{a}{2}, 0\right), \left(\frac{2a}{3}, \sqrt{\frac{3}{2a}}\right), \left(\frac{5a}{6}, -\sqrt{\frac{3}{2a}}\right), (a,0)\right\}.$$



Plot the fourth eigenstate with the $N = 10$ approximation.



Plot the fourth eigenstate with the $N = 20$ approximation.

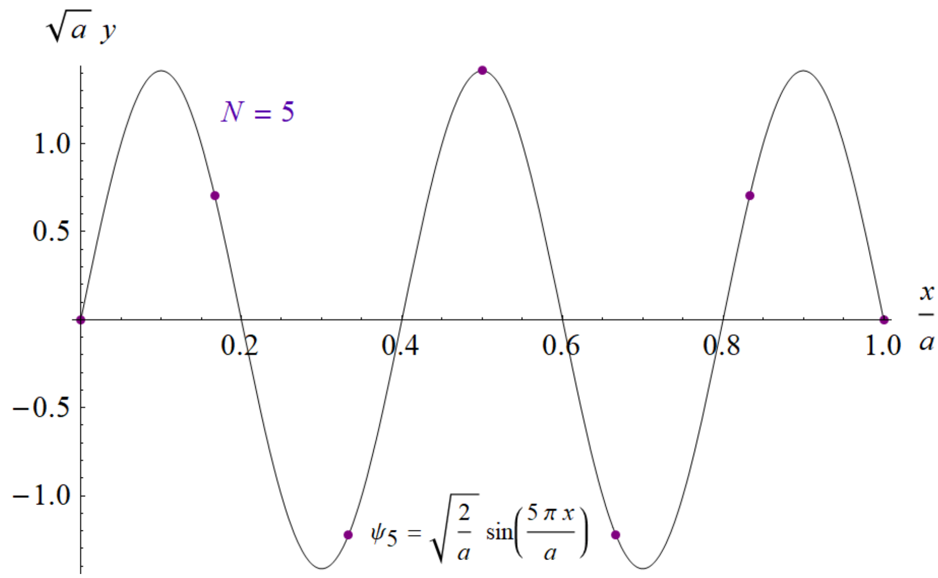


The fifth eigenstate is

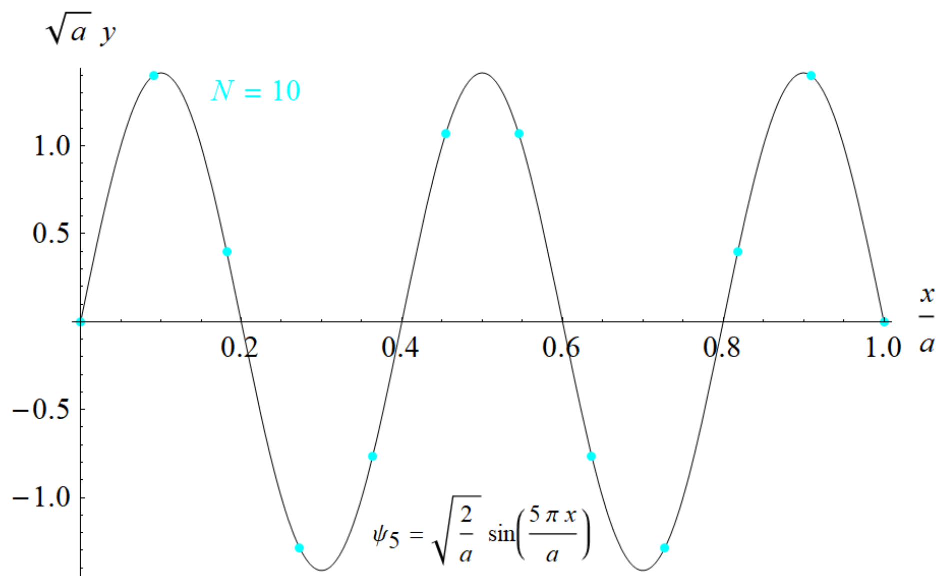
$$\psi_5(x) = \sqrt{\frac{2}{a}} \sin \frac{5\pi x}{a}.$$

Plot it together with the $N = 5$ approximation, that is, the seven points,

$$\Psi_5 = \begin{bmatrix} \frac{1}{\sqrt{2a}} \\ -\sqrt{\frac{3}{2a}} \\ \sqrt{\frac{2}{a}} \\ -\sqrt{\frac{3}{2a}} \\ \frac{1}{\sqrt{2a}} \end{bmatrix} : \qquad \left\{(0,0), \left(\frac{a}{6}, \frac{1}{\sqrt{2a}}\right), \left(\frac{a}{3}, -\sqrt{\frac{3}{2a}}\right), \left(\frac{a}{2}, \sqrt{\frac{2}{a}}\right), \left(\frac{2a}{3}, -\sqrt{\frac{3}{2a}}\right), \left(\frac{5a}{6}, \frac{1}{\sqrt{2a}}\right), (a,0)\right\}.$$



Plot the fifth eigenstate with the $N = 10$ approximation.



Plot the fifth eigenstate with the $N = 20$ approximation.