9.2. To show that the raising operator deserves its name, act with $a^\dagger$ on an energy eigenstate $|E\rangle$, and then consider what happens when the Hamiltonian H acts on $a^\dagger|E\rangle$:

$$H\left(a^\dagger|E\rangle\right) = Ha^\dagger|E\rangle$$

The commutator $\left[H, a^\dagger\right] = +\hbar\omega a^\dagger$ tells us that $Ha^\dagger = a^\dagger H + \hbar\omega a^\dagger$, so we get

$$\begin{aligned} H\left(a^\dagger|E\rangle\right) &= \left(a^\dagger H + \hbar\omega a^\dagger\right)|E\rangle \\ &= a^\dagger H|E\rangle + \hbar\omega a^\dagger|E\rangle \end{aligned}$$

Now use the energy eigenvalue equation $H|E\rangle = E|E\rangle$ to obtain

$$\begin{aligned} H\left(a^\dagger|E\rangle\right) &= a^\dagger E|E\rangle + \hbar\omega a^\dagger|E\rangle \\ &= \left(E + \hbar\omega\right)\left(a^\dagger|E\rangle\right) \end{aligned}$$

This tells us that when the new ket $a^\dagger|E\rangle$ is acted on by the Hamiltonian H, the result is the same ket $a^\dagger|E\rangle$ multiplied by the factor $(E + \hbar\omega)$, which means that the new ket $a^\dagger|E\rangle$ is also an eigenstate of H, but with an energy eigenvalue $(E + \hbar\omega)$ that is larger than the eigenvalue E of the original ket $|E\rangle$ by one quantum of energy. So $a^\dagger$ has earned its name as the "raising operator."

9.3. The unnormalized wave function is $e^{-m\omega x^2/2\hbar}$. Now normalize:

$$1 = \int_{-\infty}^{\infty}\left|\varphi_0(x)\right|^2 dx = \int_{-\infty}^{\infty}\left|Ae^{-m\omega x^2/2\hbar}\right|^2 dx = |A|^2\int_{-\infty}^{\infty} e^{-m\omega x^2/\hbar}\,dx$$

From Eq. (F.22) we get the integral, giving

$$1 = |A|^2\, 2\frac{1}{2\sqrt{m\omega/\hbar}}\sqrt{\pi} = |A|^2\sqrt{\frac{\pi\hbar}{m\omega}}$$

Choosing the normalization constant to be real and positive gives

$$\varphi_0(x) = \left(\frac{m\omega}{\pi\hbar}\right)^{1/4} e^{-m\omega x^2/2\hbar}$$

9.4. The forbidden region is beyond x_0 (or - x_0) where

$$\begin{aligned} E &= T + U = \tfrac{1}{2}m\omega^2 x_0^2 = \tfrac{1}{2}\hbar\omega \\ x_0 &= \sqrt{\frac{\hbar}{m\omega}} \end{aligned}$$

The probability of finding the particle in the forbidden region is

$$P_{|x|>x_0} = 2\int_{x_0}^{\infty} |\varphi_0(x)|^2\, dx = 2\int_{x_0}^{\infty} \left| \left(\frac{m\omega}{\pi\hbar}\right)^{1/4} e^{-m\omega x^2/2\hbar} \right|^2 dx = 2\sqrt{\frac{m\omega}{\pi\hbar}} \int_{\sqrt{\hbar/m\omega}}^{\infty} e^{-m\omega x^2/\hbar}\, dx$$

This integral can be looked up in a table and is often called the error function, defined by:

$$erf(z) = \frac{2}{\sqrt{\pi}} \int_0^z e^{-t^2}\, dt$$

$$erfc(z) = 1 - erf(z) = \frac{2}{\sqrt{\pi}} \int_z^{\infty} e^{-t^2}\, dt$$

We just need to make ours look like it. Change variables to $t = \sqrt{m\omega/\hbar}x$:

$$P_{|x|>x_0} = \frac{2}{\sqrt{\pi}} \int_1^{\infty} e^{-t^2}\, dt = erfc(1) = 1 - erf(1)$$

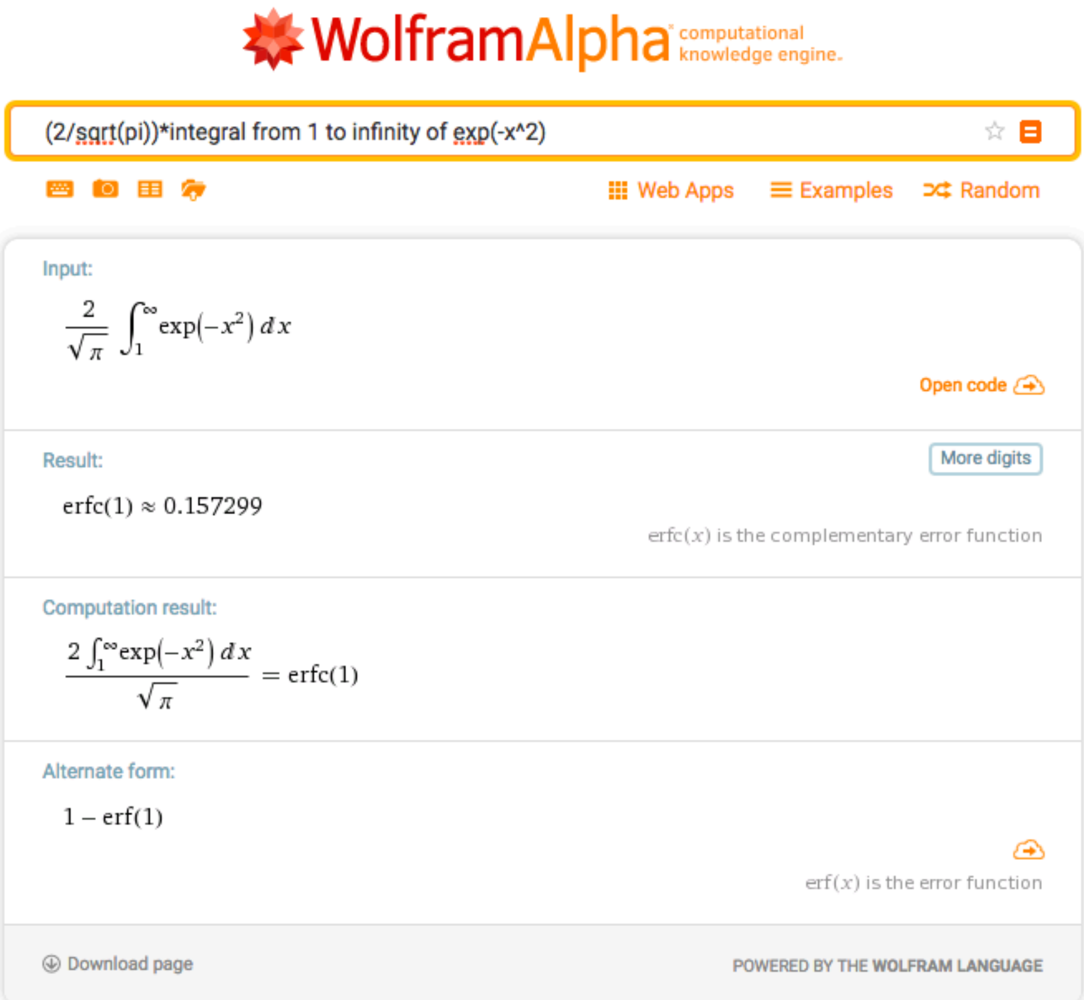
From the CRC handbook, we have

$$erfc(x) = 1 - erf(x) = 2\left(1 - F\left(\sqrt{2}x\right)\right)$$

$$F\left(\sqrt{2}\right) = 0.9213$$

$$erfc(1) = 2(1 - 0.9213) = 0.157$$

$$P_{|x|>x_0} = 0.157$$



9.10. The matrix elements of the ladder operators are given by

$$\langle m|a|n\rangle = \langle m|\sqrt{n}|n-1\rangle = \sqrt{n}\;\delta_{m,n-1} \qquad \langle m|a^\dagger|n\rangle = \langle m|\sqrt{n+1}|n+1\rangle = \sqrt{n+1}\;\delta_{m,n+1}$$

In component notation this is

$$a_{mn} = \sqrt{n}\;\delta_{m,n-1} \qquad a^\dagger_{mn} = \sqrt{n+1}\;\delta_{m,n+1}$$

with the first index labeling the row and the second the column. For example, a few elements are

$$a_{00} = \sqrt{0}\delta_{0,0-1} = 0,\; a_{01} = \sqrt{1}\delta_{0,1-1} = 1,\; a_{02} = \sqrt{2}\delta_{0,2-1} = 0,\; a_{12} = \sqrt{2}\delta_{1,2-1} = \sqrt{2}$$
$$a^\dagger_{00} = \sqrt{0+1}\;\delta_{0,0+1} = 0,\; a^\dagger_{01} = \sqrt{1+1}\;\delta_{0,1+1} = 0,\; a^\dagger_{10} = \sqrt{0+1}\;\delta_{1,0+1} = 1$$

The explicit matrix representations are

$$a \doteq \begin{pmatrix} a_{00} & a_{01} & a_{02} & a_{03} & \cdots \\ a_{10} & a_{11} & a_{12} & a_{13} & \cdots \\ a_{20} & a_{21} & a_{22} & a_{23} & \cdots \\ a_{30} & a_{31} & a_{32} & a_{33} & \cdots \\ \vdots & \vdots & \vdots & \vdots & \ddots \end{pmatrix} \qquad a^\dagger \doteq \begin{pmatrix} a^\dagger_{00} & a^\dagger_{01} & a^\dagger_{02} & a^\dagger_{03} & \cdots \\ a^\dagger_{10} & a^\dagger_{11} & a^\dagger_{12} & a^\dagger_{13} & \cdots \\ a^\dagger_{20} & a^\dagger_{21} & a^\dagger_{22} & a^\dagger_{23} & \cdots \\ a^\dagger_{30} & a^\dagger_{31} & a^\dagger_{32} & a^\dagger_{33} & \cdots \\ \vdots & \vdots & \vdots & \vdots & \ddots \end{pmatrix}$$

Using the equations above, we get the matrix representations

$$a \doteq \begin{pmatrix} 0 & \sqrt{1} & 0 & 0 & \cdots \\ 0 & 0 & \sqrt{2} & 0 & \cdots \\ 0 & 0 & 0 & \sqrt{3} & \cdots \\ 0 & 0 & 0 & 0 & \cdots \\ \vdots & \vdots & \vdots & \vdots & \ddots \end{pmatrix} \qquad a^\dagger \doteq \begin{pmatrix} 0 & 0 & 0 & 0 & \cdots \\ \sqrt{1} & 0 & 0 & 0 & \cdots \\ 0 & \sqrt{2} & 0 & 0 & \cdots \\ 0 & 0 & \sqrt{3} & 0 & \cdots \\ \vdots & \vdots & \vdots & \vdots & \ddots \end{pmatrix}$$

9.17 a) Before we do any calculations we must normalize the state. Let's use Dirac notation to simplify the calculations.

$$|\psi(0)\rangle = A\left[|0\rangle + 2|1\rangle + 2|2\rangle\right]$$

$$1 = \langle\psi(0)|\psi(0)\rangle = A^*\left[\langle 0| + 2\langle 1| + 2\langle 2|\right]A\left[|0\rangle + 2|1\rangle + 2|2\rangle\right]$$

$$= |A|^2\left[\langle 0|0\rangle + 4\langle 1|1\rangle + 4\langle 2|2\rangle\right] = |A|^2\,9 \qquad \Rightarrow A = \tfrac{1}{3}$$

We are free to choose A to be real and positive because an overall phase is not physical. Now let's find the time dependent state vector. The component states are energy eigenstates, so we simply multiply by the appropriate phase factors:

$$|\psi(0)\rangle = \tfrac{1}{3}\left(|0\rangle + 2|1\rangle + 2|2\rangle\right)$$

$$|\psi(t)\rangle = \tfrac{1}{3}\left(e^{-i\frac{E_0}{\hbar}t}|0\rangle + 2e^{-i\frac{E_1}{\hbar}t}|1\rangle + 2e^{-i\frac{E_2}{\hbar}t}|2\rangle\right) = \tfrac{1}{3}\left(e^{-i\frac{\omega}{2}t}|0\rangle + 2e^{-i\frac{3\omega}{2}t}|1\rangle + 2e^{-i\frac{5\omega}{2}t}|2\rangle\right)$$

$$= \tfrac{1}{3}e^{-i\frac{\omega}{2}t}\left(|0\rangle + 2e^{-i\omega t}|1\rangle + 2e^{-i2\omega t}|2\rangle\right)$$

Because there are three energy eigenstates in the state vector, there are three possible energies $E_n = \left(n + \tfrac{1}{2}\right)\hbar\omega$ that can be measured: $E_0 = \tfrac{1}{2}\hbar\omega$, $E_1 = \tfrac{3}{2}\hbar\omega$, $E_2 = \tfrac{5}{2}\hbar\omega$. The probabilities are

$$\mathsf{P}_{E_n} = \left|\langle n|\psi(t)\rangle\right|^2 = \left|\langle n|\tfrac{1}{3}e^{-i\frac{\omega}{2}t}\left(|0\rangle + 2e^{-i\omega t}|1\rangle + 2e^{-i2\omega t}|2\rangle\right)\right|^2$$

$$\boxed{\begin{aligned} \mathsf{P}_{E_0} &= \left(\tfrac{1}{3}\right)^2 = \tfrac{1}{9} = 0.11\overline{1} \\ \mathsf{P}_{E_1} &= \left(\tfrac{2}{3}\right)^2 = \tfrac{4}{9} = 0.44\overline{4} \\ \mathsf{P}_{E_2} &= \left(\tfrac{2}{3}\right)^2 = \tfrac{4}{9} = 0.44\overline{4} \end{aligned}}$$

The energy states are stationary states, so this result is time independent.

b) To find the expectation value of the momentum, use ladder operators rather than doing spatial integrals.

$$\begin{aligned} \langle p\rangle &= \langle\psi(t)|p|\psi(t)\rangle = i\sqrt{\frac{m\omega\hbar}{2}}\langle\psi(t)|a^\dagger - a|\psi(t)\rangle \\ &= i\sqrt{\frac{m\omega\hbar}{2}}\tfrac{1}{3}e^{+i\frac{\omega}{2}t}\left[\langle 0| + 2e^{+i\omega t}\langle 1| + 2e^{+i2\omega t}\langle 2|\right]\left(a^\dagger - a\right)\tfrac{1}{3}e^{-i\frac{\omega}{2}t}\left[|0\rangle + 2e^{-i\omega t}|1\rangle + 2e^{-i2\omega t}|2\rangle\right] \\ &= i\sqrt{\frac{m\omega\hbar}{2}}\tfrac{1}{9}\left[-2e^{-i\omega t}\langle 0|a|1\rangle - 4e^{-i\omega t}\langle 1|a|2\rangle + 2e^{+i\omega t}\langle 1|a^\dagger|0\rangle + 4e^{+i\omega t}\langle 2|a^\dagger|1\rangle\right] \\ &= i\sqrt{\frac{m\omega\hbar}{2}}\tfrac{1}{9}\left[-2\sqrt{1}e^{-i\omega t} - 4\sqrt{2}e^{-i\omega t} + 2\sqrt{1}e^{+i\omega t} + 4\sqrt{2}e^{+i\omega t}\right] \\ &= i\sqrt{\frac{m\omega\hbar}{2}}\tfrac{1}{9}\left(2 + 4\sqrt{2}\right)\left(e^{+i\omega t} - e^{-i\omega t}\right) \end{aligned}$$

$$\boxed{\langle p\rangle = -\sqrt{\frac{m\omega\hbar}{2}}\tfrac{4}{9}\left(1 + 2\sqrt{2}\right)\sin\omega t}$$

c) Here again, Dirac notation is simpler. The energy states are stationary states, so this result is time independent.

$$\begin{aligned} \langle E\rangle &= \langle\psi|H|\psi\rangle = \tfrac{1}{3}\left[\langle 0| + 2\langle 1| + 2\langle 2|\right]H\tfrac{1}{3}\left[|0\rangle + 2|1\rangle + 2|2\rangle\right] \\ &= \tfrac{1}{9}\left[\langle 0|H|0\rangle + 4\langle 1|H|1\rangle + 4\langle 2|H|2\rangle\right] = \tfrac{1}{9}\left[\tfrac{1}{2}\hbar\omega + 4\tfrac{3}{2}\hbar\omega + 4\tfrac{5}{2}\hbar\omega\right] = \tfrac{33}{18}\hbar\omega \end{aligned}$$

$$\boxed{\langle E\rangle = \tfrac{11}{6}\hbar\omega \cong 1.83\ \hbar\omega}$$

The same result is obtained with the probability weighting method:

$$\langle E\rangle = \sum_n E_n\mathsf{P}_{E_n} = \tfrac{1}{2}\hbar\omega\tfrac{1}{9} + \tfrac{3}{2}\hbar\omega\tfrac{4}{9} + \tfrac{5}{2}\hbar\omega\tfrac{4}{9} = \tfrac{33}{18}\hbar\omega = \tfrac{11}{6}\hbar\omega$$

d) Now find the standard deviation of the energy.

$$\Delta E = \sqrt{\left\langle \left(E - \langle E\rangle\right)^2 \right\rangle} = \sqrt{\left\langle E^2 - 2E\langle E\rangle + \langle E\rangle^2 \right\rangle} = \sqrt{\left\langle E^2 \right\rangle - \langle E\rangle^2}$$

$$\left\langle E^2 \right\rangle = \langle \psi | H^2 | \psi \rangle = \tfrac{1}{3}\left[\langle 0| + 2\langle 1| + 2\langle 2|\right] H^2 \tfrac{1}{3}\left[|0\rangle + 2|1\rangle + 2|2\rangle\right]$$

$$\left\langle E^2 \right\rangle = \tfrac{1}{9}\left[\langle 0|H^2|0\rangle + 4\langle 1|H^2|1\rangle + 4\langle 2|H^2|2\rangle\right] = \tfrac{1}{9}\left[\left(\tfrac{1}{2}\hbar\omega\right)^2 + 4\left(\tfrac{3}{2}\hbar\omega\right)^2 + 4\left(\tfrac{5}{2}\hbar\omega\right)^2\right]$$

$$\left\langle E^2 \right\rangle = \tfrac{137}{36}\hbar^2\omega^2$$

$$\Delta E = \sqrt{\tfrac{137}{36}\hbar^2\omega^2 - \left(\tfrac{33}{18}\right)^2 \hbar^2\omega^2} = \hbar\omega\sqrt{\tfrac{144}{18^2}}$$

$$\boxed{\Delta E = \tfrac{2}{3}\hbar\omega}$$

```
%*****************************************************************
% Program 4: Find several lowest eigenmodes V(x) and
% eigenenergies E of 1D Schrodinger equation
% -1/2*hbar^2/m(d2/dx2)V(x) + U(x)V(x) = EV(x)
% for arbitrary potentials U(x)
%*****************************************************************
% Parameters for solving problem in the interval -L < x < L

% PARAMETERS:
L = 5;
N = 1000;
x = linspace(-L,L,N)';
dx = x(2) - x(1);

U = 1/2*100*x.^(2); % quadratic harmonic oscillator potential

% Three-point finite-difference representation of Laplacian
% using sparse matrices, where you save memory by only
% storing non-zero matrix elements

e = ones(N,1);
Lap = spdiags([e -2*e e],[-1 0 1],N,N)/dx^2;

% Total Hamiltonian
hbar = 1; m = 1; % constants for Hamiltonian

H = -1/2*(hbar^2/m)*Lap + spdiags(U,0,N,N);
%H = -1/2*(hbar^2/m)*D_2 + spdiags(U,0,N,N);

% Find lowest nmodes eigenvectors and eigenvalues of sparse matrix
nmodes = 4; opts.disp = 0;
[V,E] = eigs(H,nmodes,'sa',opts);        % find eigs
```

```
[E,ind] = sort(diag(E));          % convert E to vector and sort low to high
V = V(:,ind);                     % rearrange corresponding eigenvectors

% Generate plot of lowest energy eigenvectors V(x) and U(x)

Usc = U*max(abs(V(:)))/max(abs(U));
% rescale U for plotting

plot(x,V,x,Usc,'--k');        % plot V(x) and rescaled U(x)
% Add legend showing Energy of plotted V(x)

lgnd_str = [repmat('E = ',nmodes,1),num2str(E)];

legend(lgnd_str) % place legend string on plot
shg
```