Q1 a)

$\frac{E_n}{E_1^{(0)}}$ Plot for:

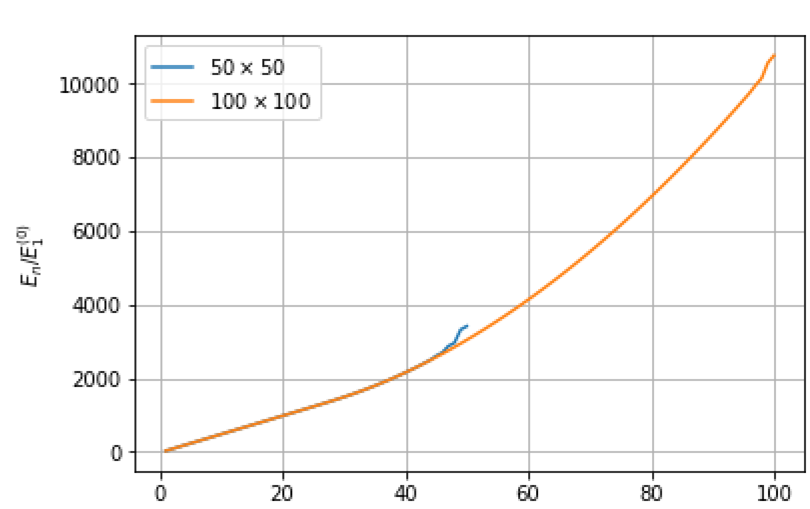
$$\frac{H_{ij}}{E_1^{(0)}} = \delta_{ij}\left\{j^2 + \frac{\pi^2\rho^2}{48}\left(1 - \frac{6}{(\pi j)^2}\right)\right\} + [1-\delta_{ij}]\left\{\frac{\rho^2}{2}\frac{(-1)^{i+j}+1}{2}\left(\frac{1}{(i-j)^2} - \frac{1}{(i+j)^2}\right)\right\}$$

In [49]:

```
import numpy as np
import scipy.linalg as la
import matplotlib.pyplot as plt

def eigenstate(size):
    rho = 50
    v = np.pi**2*rho**2/48
    delta = np.identity(size)

    n = 0
    m = 0
    matrix1 = np.zeros((size, size))

    while n < size:
        while m < size:
            elem = (m+1)**2+v*(1 - 6/(np.pi*(m+1))**2)
            matrix1[n, m] = delta[n, m] * elem
            m = m+1
        m = 0
        n = n + 1

    matrix2 = np.zeros((size, size))
    n = 0
    m = 0
    while n < size:
        while m < size:

            if m != n:
                elem = 0.25*rho**2*((-1)**(m+n+2)+1)*(1/(n-m)**2-1/(n+m+2)**2)
            else:
                elem = 0

            matrix2[n, m] = (1-delta[n, m]) * elem
            m = m+1
        m = 0
        n = n + 1

    matrix = matrix1 + matrix2
    eigenValues, eigenVectors = la.eig(matrix)
    eigenValues = np.real(eigenValues)

    idx = eigenValues.argsort()[::1]
    eigenValues = eigenValues[idx]
    eigenVectors = eigenVectors[:,idx]

    index = np.linspace(1, size, size)
    return index, eigenValues, eigenVectors


n50, e50, eve50 = eigenstate(50)
plt.plot(n50, e50, label = r'$50 \times 50$')
n100, e100, eve100 = eigenstate(100)
plt.plot(n100, e100, label = r'$100 \times 100$')
plt.legend()
plt.grid()
plt.xlabel("n")
plt.ylabel(r'${E_{n}}/{E_{1}^{(0)}}$')
```

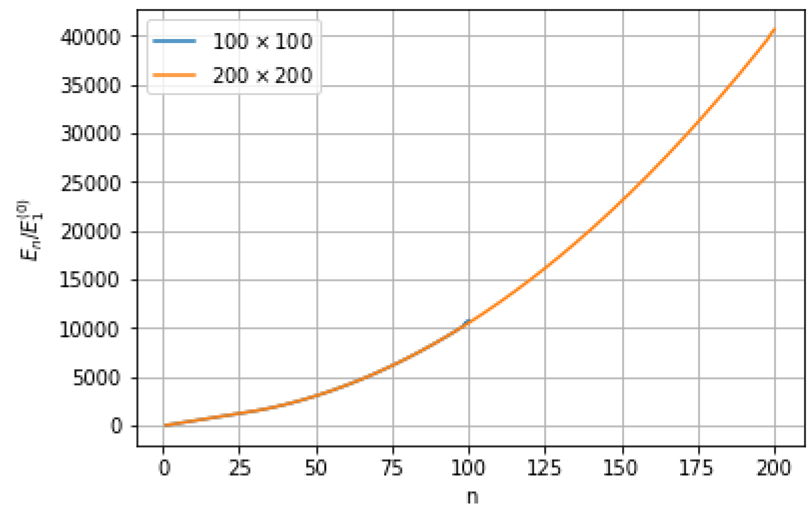
Out[49]:

```
Text(0,0.5,'${E_{n}}/{E_{1}^{(0)}}$')
```



Truncation error shows up around the $n = 50$ for 50×50 matrixes.

In [50]:
```
n100, e100, eve100 = eigenstate(100)
plt.plot(n100, e100, label = r'$100 \times 100$')
n200, e200, eve200 = eigenstate(200)
plt.plot(n200, e200, label = r'$200 \times 200$')
plt.xlabel("n")
plt.ylabel(r'${E_{n}}/{E_{1}^{(0)}}$')
plt.legend()
plt.grid()
```

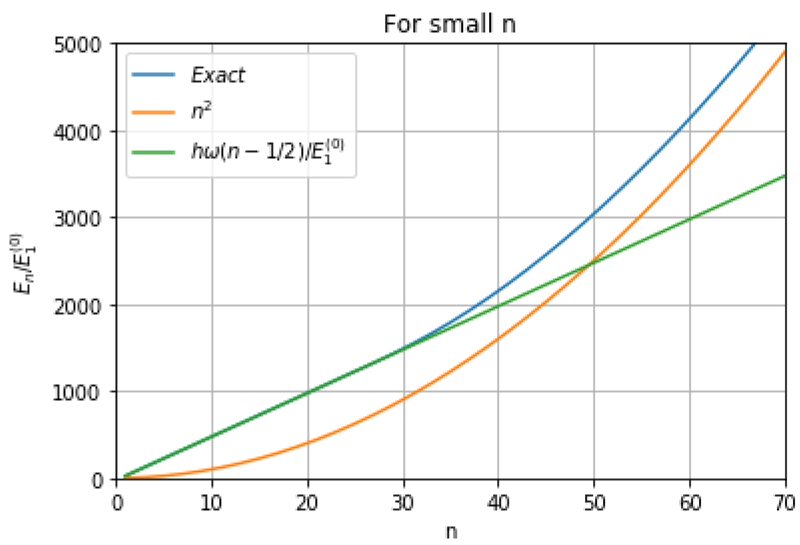


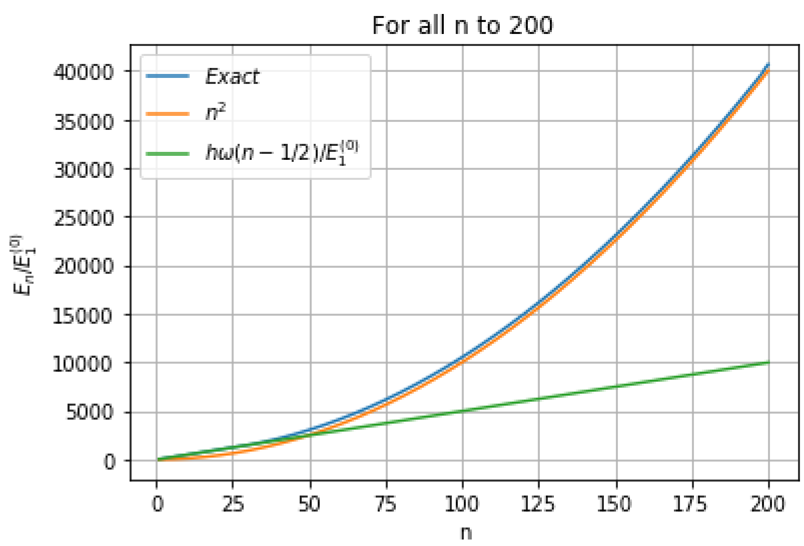
Truncation error shows up around the $n = 100$ for 100×100 matrixes, but relatively smaller.

The energy ratio for harmonic oscillator is $\frac{h\omega(n-1/2)}{E_1^{(0)}}$. Harmonic oscillator n start from 0 as ground state.

The energy for infinite square well is $E_n = \frac{n^2\pi^2\hbar^2}{2ma^2}$, so energy ratio will be $\frac{E_n}{E_1} = n^2$

In [52]:
```
sho = 50*((n200)-1/2) # since n400 start from 1, but harmonic oscillator n start from 0
inf_sq = n200**2

plt.plot(n200, e200, label = r'$Exact$')
plt.plot(n200, inf_sq, label = r'$n^{2}$' )
plt.plot(n200, sho, label = r'$h\omega(n-1/2)/E_1^{(0)}$')
plt.xlim(0, 70)
plt.ylim(0, 5000)
plt.title('For small n')
plt.xlabel("n")
plt.ylabel(r'${E_{n}}/{E_{1}^{(0)}}$')
plt.legend()
plt.grid()

plt.figure()
plt.plot(n200, e200, label = r'$Exact$')
plt.plot(n200, inf_sq, label = r'$n^{2}$' )
plt.plot(n200, sho, label = r'$h\omega(n-1/2)/E_1^{(0)}$')
plt.xlabel("n")
plt.ylabel(r'${E_{n}}/{E_{1}^{(0)}}$')
plt.title('For all n to 200')
plt.legend()
plt.grid()
```

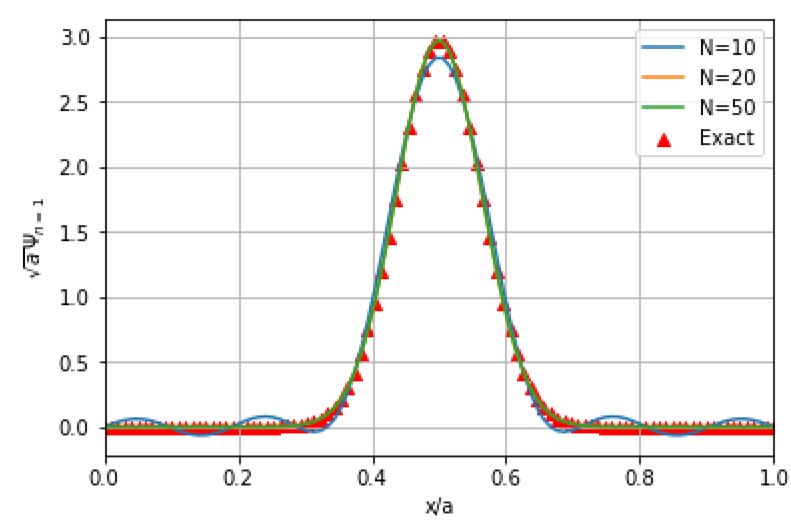




Q1 b) i)

$N_{max} = 10; 20; 50$ plot:

In [79]:
```
def numerical(eigenV, order):
    x = np.linspace(0, 1, 100)
    n = 1
    psi = 0
    while n < order:
        basis = np.sqrt(2)*np.sin(n*np.pi*x)
        ci = eigenV[n-1]
        psi = psi+ basis*ci
        n = n+1
    return x, psi

x_n, psi_10 = numerical(eve50[:, 0], 10)
x_n, psi_20 = numerical(eve50[:, 0], 20)
x_n, psi_50 = numerical(eve50[:, 0], 50)

x = x_n
psi = (np.pi/2*50)**0.25*np.exp(-np.pi**2/4*50*(x-0.5)**2)

plt.figure()
plt.scatter(x, psi, marker='^', c = 'red', label = 'Exact')
plt.plot(x_n, psi_10, label = 'N=10')
plt.plot(x_n, psi_20, label = 'N=20')
plt.plot(x_n, psi_50, label = 'N=50')
plt.xlabel("x/a")
plt.ylabel(r'$\sqrt{a}\Psi_{n=1}$')
plt.xlim(0, 1)
plt.legend()
plt.grid()
```



Q1 b) ii)

First excited state for harmonic oscillator:

$$\sqrt{a}\psi_1(x) = \left(\frac{\pi}{2}\frac{\hbar\omega}{E_1^{(0)}}\right)^{3/4}\sqrt{2\pi}\left(\frac{x}{a}-\frac{1}{2}\right)e^{-\frac{\pi^2}{4}\frac{\hbar\omega}{E_1^{(0)}}\left(\frac{x}{a}-\frac{1}{2}\right)^2}$$

In [80]:
```
psi2 = (np.pi/2*50)**0.75*np.sqrt(2*np.pi)*(x-1/2)*np.exp(-np.pi**2/4*50*(x-0.5)**2)
plt.scatter(x, psi2, marker='^', c = 'red', label = 'Exact')

x_n, psi2_10 = numerical(-eve50[:, 1], 10)
x_n, psi2_20 = numerical(-eve50[:, 1], 20)
x_n, psi2_50 = numerical(-eve50[:, 1], 50)
#plt.scatter(x, psi, marker='^', c = 'red', label = 'Exact')
plt.plot(x_n, psi2_10, label = 'N=10')
plt.plot(x_n, psi2_20, label = 'N=20')
plt.plot(x_n, psi2_50, label = 'N=50')
plt.xlabel("x/a")
plt.ylabel(r'$\sqrt{a}\Psi_{n=2}$')
plt.xlim(0, 1)
plt.legend()
plt.grid()
```