Q2b)

Since

$$K_{ij} = j^2 E_1^{(0)} \delta_{ij}$$
$$V_{ij} = \lambda \tfrac{2}{a} \int_0^a dx \sin\left(\tfrac{i\pi x}{a}\right)\left(x - \tfrac{a}{2}\right)^4 \sin\left(\tfrac{j\pi x}{a}\right)$$

First define

$$J_4(n) = \int_0^1 du(u - 1/4)cos(\pi a u)$$

Rewritten as delta

$$J_4(n) = \delta_{n,0}\frac{1}{80} + (1 - \delta_{n,0})\,\frac{1 + (-1)^n}{2}\left(\frac{1}{(n\pi)^2} - \frac{24}{(n\pi)^4}\right)$$

That

$$V_{ij} = \lambda a^4 \left[J_4(i-j) - J_4(i+j)\right] \equiv \lambda a^4 F_{ij}$$

And the matrix

$$\frac{H_{ij}}{E_1^{(0)}} = j^2 \delta_{ij} + \lambda a^4 \frac{2m_0}{\hbar^2}\frac{a^2}{\pi^2} F_{ij} = j^2 \delta_{ij} + \pi^4 s^6 F_{ij}$$

Construct the matrix in code:

In [2]:
```
import numpy as np
import matplotlib.pyplot as plt
import scipy.linalg as la


def delta(m, n):
    if n == m:
        delta = 1
    else:
        delta = 0
    return delta


def j4(n):
    if n == 0:
        return 1/80
    else:
        return (1+(-1)**n)/2*(1/(n*np.pi)**2 - 24/(n*np.pi)**4)


def fij(i, j):
    return j4(i-j) - j4(i+j)

def isw(s, size): #### infinite square well basis
    i = 0
    hij = np.zeros((size, size))
    while i < size:
        j = 0
        while j < size:
            elem = (j+1)**2*delta(i+1, j+1) + np.pi**4*s**6*fij(i+1, j+1)
            hij[i, j] = elem
            j = j+1
        i = i+1

    eigenValues, eigenVectors = la.eig(hij)
    eigenValues = np.real(eigenValues)

    index = np.linspace(0, size, size)

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

    return eigenValues, eigenVectors, index

es1, evs1, ns1 = isw(1, 800)
es2, evs2, ns2 = isw(2, 800)
es5, evs5, ns5 = isw(5, 800)
es10, evs10, ns10 = isw(10, 800)
```

Since energy

$$E_n = \left(\frac{\hbar^2}{2m_0}\right)^{2/3} \lambda^{1/3} \frac{\epsilon_n}{s^2}$$

The coefficient $\frac{\epsilon_n}{s^2}$ is determined as:

In [3]:
```
print('When s = 1, E0/e0 = ', es1[0]/1)
print('When s = 2, E0/e0 = ', es2[0]/2**2)
print('When s = 5, E0/e0 = ', es5[0]/5**2)
print('When s = 10, E0/e0 = ', es10[0]/10**2)
```

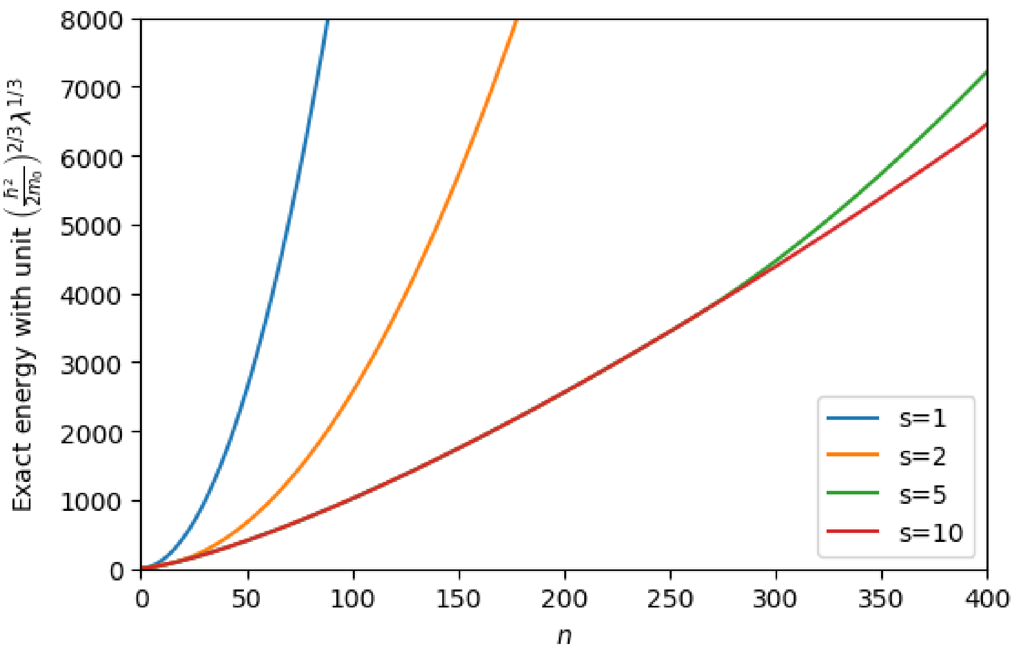
```
When s = 1, E0/e0 =  1.2254173873316159
When s = 2, E0/e0 =  1.0603620940347849
When s = 5, E0/e0 =  1.060362090487117
When s = 10, E0/e0 =  1.06036209047772
```

c)

Plot the exact energy with the unit $\left(\frac{\hbar^2}{2m_0}\right)^{2/3}\lambda^{1/3}$

In [12]:
```
plt.figure(dpi=100)
plt.plot(ns1, es1/1, label = 's=1')
plt.plot(ns2, es2/2**2, label = 's=2')
plt.plot(ns5, es5/5**2, label = 's=5')
plt.plot(ns10, es10/10**2, label ='s=10')
plt.xlim(0, 400)
plt.ylim(0, 8000)
plt.ylabel(r'Exact energy with unit $\left(\frac{\hbar^{2}}{2 m_{0}}\right)^{2 / 3} \lambda^{1 / 3}$')
plt.xlabel(r'$n$')
plt.legend()
```

Out[12]: <matplotlib.legend.Legend at 0x7ff82376aa58>



For the overlaping $s = 5$ and $s = 10$ energy (n less than around 250), is the results indicative λx^4 potential. As the energy goes up, the effect of potential shows up again cause the division.

d)

Consider $V = \lambda(x-1/2)^4$ as perturbation $H' = \lambda(x-1/2)^4$, then:

$$E_n^{(0)} = \langle n|\lambda(x-1/2)^4|n\rangle$$

Since

$$V_{ij} = \lambda\frac{2}{a}\int_0^a dx \sin\left(\frac{i\pi x}{a}\right)\left(x-\frac{a}{2}\right)^4 \sin\left(\frac{j\pi x}{a}\right) = \lambda a^4\left[J_4(i-j) - J_4(i+j)\right] \equiv \lambda a^4 F_{ij}$$

Therefore

$$\langle n|\lambda(x-1/2)^4|n\rangle = \lambda a^4\left[J_4(0) - J_4(2n)\right] = \frac{\lambda a^4}{80}$$

$\lambda a^4 \frac{2m_0}{\hbar^2}\frac{a^2}{\pi^2} = \pi^4 s^6 \rightarrow a^4 = \left(\frac{\hbar}{2m}\right)^{2/3}\lambda^{-2/3}\pi^4 s^4$, so

$$E_n^{(1)} = \frac{\lambda a^4}{80} = \left(\frac{\hbar}{2m}\right)^{2/3}\lambda^{1/3}\pi^4 s^4\left(\frac{1}{80} - \frac{1}{4n^2\pi^2} + \frac{3}{2n^4\pi^4}\right)$$

So

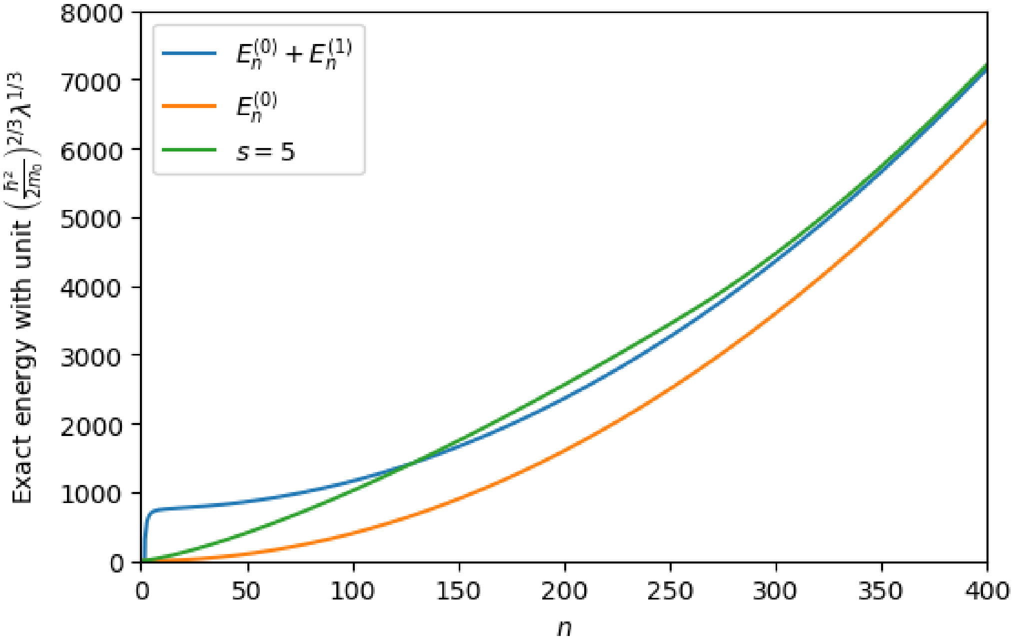
$$E_n^{(0)} + E_n^{(1)} = \left(\frac{\hbar}{2m}\right)^{2/3}\lambda^{1/3}\left(\frac{n^2}{s^2} + \frac{\pi^4 s^4}{80} - \frac{\pi^4 s^4}{4n^2\pi^2} + \frac{3\pi^4 s^4}{2n^4\pi^4}\right)$$

As n goes large, $\frac{\pi^4 s^4}{4n^2\pi^2}$ and $\frac{3\pi^4 s^4}{2n^4\pi^4}$ terms vanish.

In [11]:
```
plt.figure(dpi=100)
En0 = ns5**2/5**2
En1 = np.pi**4*5**4*(1/80-(1/(4*ns5**2*np.pi**2) +3/(2*ns5**4*np.pi**4)))
plt.plot(ns5, En0+En1, label = r'$E_n^{(0)}+E_n^{(1)}$')
plt.plot(ns5, En0, label = r'$E_n^{(0)}$')
plt.xlim(0, 400)
plt.ylim(0, 8000)
plt.plot(ns5, es5/5**2, label = r'$s=5$')
plt.legend()
plt.ylabel(r'Exact energy with unit $\left(\frac{\hbar^{2}}{2 m_{0}}\right)^{2 / 3} \lambda^{1 / 3}$')
plt.xlabel(r'$n$')
```

```
/home/alex/.local/lib/python3.6/site-packages/ipykernel_launcher.py:3: RuntimeWarning: divide by zero encountered in true_divide
  This is separate from the ipykernel package so we can avoid doing imports until
```

Out[11]: Text(0.5,0,'n')



e)

Since $\alpha \equiv m_0\omega/\hbar$ and $\alpha = \left(\frac{6\lambda m_0}{\hbar^2}\right)^{1/3}$ from part (a), we have

$$\frac{m_0\omega}{\hbar} = \left(\frac{6\lambda m_0}{\hbar^2}\right)^{1/3}$$

Get $\lambda = \frac{m_0^2 w^3}{6\hbar}$ and $\hbar\omega = 2\left(3^{1/3}\right)\left(\frac{\hbar^2}{2m_0}\right)^{2/3}\lambda^{1/3}$. Therefore, in order to consist with (b), define energy unit to be

$$E_0 = \frac{hw}{2\left(3^{1/3}\right)} = \left(\frac{\hbar^2}{2m_0}\right)^{2/3}\lambda^{1/3}$$

$H_{ij} \equiv \langle i|\hat{H}|j\rangle = \langle i|K|j\rangle + \langle i|V|j\rangle$

Where

$$\langle K\rangle = -\langle i|\frac{p^2}{2m_0}|j\rangle = -\frac{1}{2m_0}\langle i|p^2|j\rangle$$

Since $\hat{p} = i\sqrt{\frac{\hbar m\omega}{2}}\left(a^\dagger - a\right)$, that $\hat{p}^2 = -\frac{\hbar m\omega}{2}\left(a^\dagger a^\dagger + aa - aa^\dagger - a^\dagger a\right)$

Therefore

$$\langle K\rangle = \frac{1}{2m_0}\left\langle i\left|p^2\right|j\right\rangle = -\frac{\hbar\omega}{4}\left[\sqrt{(j+2)(j+1)}\delta_{i,j+2} + \sqrt{j(j-1)}\delta_{i,j-2} - (2j+1)\delta_{i,j}\right]$$

For $\langle V\rangle$

$$\langle V\rangle = \langle i|\lambda x^4|j\rangle$$

Where $\hat{x} = \sqrt{\frac{\hbar}{2m\omega}}\left(a^\dagger + a\right)$, that $\hat{x}^4 = \left(\frac{\hbar}{2m\omega}\right)^2\left(a^\dagger + a\right)^4$

Subsituted $\lambda = \frac{m_0^2 w^3}{6\hbar}$ in, we get

$$\langle V\rangle = \frac{hw}{24}\langle i|\left(a^\dagger + a\right)\left(a^\dagger + a\right)\left(a^\dagger + a\right)\left(a^\dagger + a\right)|j\rangle$$

Divide $E_0 = \frac{\hbar w}{2(3^{1/3})}$ to construct a dimensionless matrix.

$$H_{ij}/E_0 = -\frac{3^{1/3}}{2}\left[\sqrt{(j+2)(j+1)}\delta_{i,j+2} + \sqrt{j(j-1)}\delta_{i,j-2} - (2j+1)\delta_{ij}\right] + \frac{3^{1/3}}{12}v_{i,j}$$

Where v_{ij} is

$$
\begin{aligned}
v_{ij} =& \langle i|[a^\dagger a^\dagger + aa + (2a^\dagger a + 1)][a^\dagger a^\dagger + aa + (2a^\dagger a + 1)]|j\rangle \\
=& \sqrt{(j+4)(j+3)(j+2)(j+1)}\delta_{i,j+4} \\
&+ \sqrt{j(j-1)(j-1)j}\delta_{i,j} \\
&+ 2\sqrt{(j+2)(j+1)jj}\delta_{i,j+2} + \sqrt{(j+2)(j+1)}\delta_{i,j+2} \\
&+ \sqrt{(j+1)(j+2)(j+2)(j+1)}\delta_{i,j} \\
&+ \sqrt{(j-3)(j-2)(j-1)j}\delta_{i,j-4} \\
&+ 2\sqrt{(j-1)jjj}\delta_{i,j-2} + \sqrt{(j-1)j}\delta_{i,j-2} \\
&+ 2\sqrt{(j+2)(j+2)(j+2)(j+1)}\delta_{i,j+2} + \sqrt{(j+2)(j+1)}\delta_{i,j+2} \\
&+ 2\sqrt{(j-2)(j-2)(j-1)j}\delta_{i,j-2} + \sqrt{(j-1)j}\delta_{i,j-2} \\
&+ 4j^2\delta_{i,j} + 4j\delta_{i,j} + \delta_{i,j}
\end{aligned}
$$

Then put the H_{ij}/E_0 to the program below:

In [6]:
```
def qho(size):

    i = 0
    kij = np.zeros((size, size))

    ij1 = np.zeros((size, size))
    ij2_m = np.zeros((size, size))
    ij2_p = np.zeros((size, size))
    ij4_m = np.zeros((size, size))
    ij4_p = np.zeros((size, size))
    while i < size:
        j = 0
        while j < size:
            kij[i, j] = -(3**(1/3))/2*(np.sqrt((j+2)*(j+1))*delta(i, j+2)+np.sqrt(j*(j-1))*delta(i
, j-2) - (2*j+1)*delta(i,j))

            ij4_p[i, j] = np.sqrt((j+1)*(j+2)*(j+3)*(j+4))*delta(i, j+4)
            ij4_m[i, j] = np.sqrt((j)*(j-1)*(j-2)*(j-3))*delta(i, j-4)

            ij2_p[i, j] = (np.sqrt(j**2*(j+2)*(j+1))+np.sqrt((j+2)*(j+1))+np.sqrt((j+2)**3*(j+1)))
*2*delta(i,j+2)
            ij2_m[i, j] = (np.sqrt( (j-2)**2*(j-1)*j ) + np.sqrt( (j-1)*j ) + np.sqrt( (j-1)*j**3)
)*2*delta( i,j-2 )

            ij1[i, j] = (4*(j**2+j)+ 1 + (j+1)*(j+2) + j*(j-1) )*delta(i, j)


            j = j+1
        i = i+1

    vij = (ij4_p + ij4_m + ij2_p + ij2_m + ij1)*3**(1/3)/12
    hij = vij + kij
    eigenValues, eigenVectors = la.eig(hij)
    eigenValues = np.real(eigenValues)

    index = np.linspace(0, size-1, size)

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

    return hij, eigenValues, eigenVectors, index

hij1, eigenValues1, eigenVectors1, index1 = qho(1)
hij2, eigenValues2, eigenVectors2, index2 = qho(2)
hij5, eigenValues5, eigenVectors5, index5 = qho(5)
hij10, eigenValues10, eigenVectors10, index10 = qho(10)
hij20, eigenValues20, eigenVectors20, index20 = qho(20)
hij50, eigenValues50, eigenVectors50, index50 = qho(50)
```

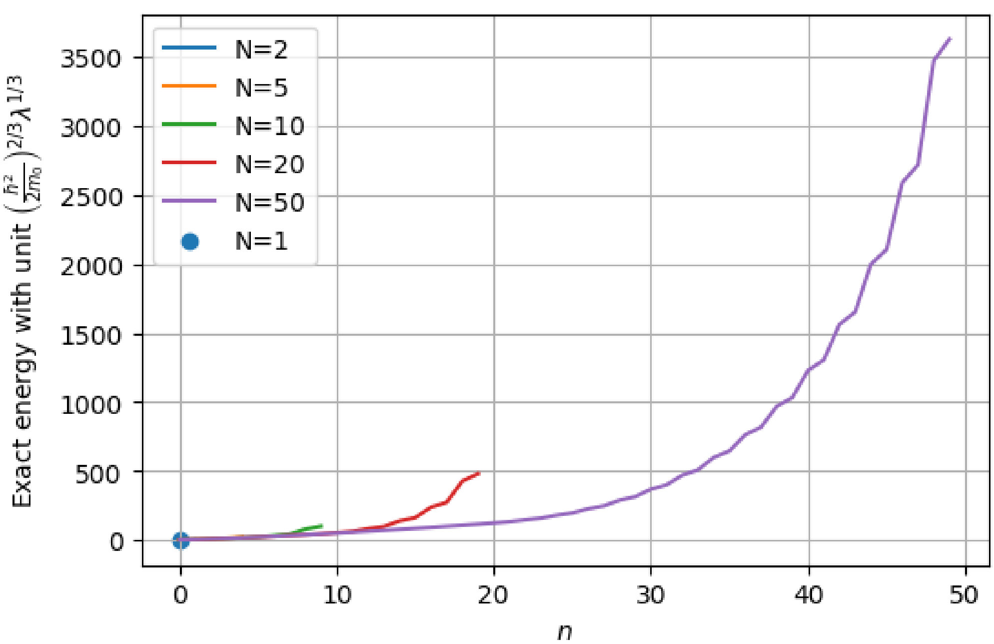
The ground state energy with the unit of $E_0 = \left(\frac{\hbar^2}{2m_0}\right)^{2/3}\lambda^{1/3}$ is shown as:

In [7]:
```
print('When N = 1, En/e0 = ', eigenValues1[0])
print('When N = 2, En/e0 = ', eigenValues2[0])
print('When N = 5, En/e0 = ', eigenValues5[0])
print('When N = 10, En/e0 = ', eigenValues10[0])
print('When N = 20, En/e0 = ', eigenValues20[0])
print('When N = 50, En/e0 = ', eigenValues50[0])
```

```
When N = 1, En/e0 =  1.0816871777305561
When N = 2, En/e0 =  1.0816871777305561
When N = 5, En/e0 =  1.0631238922817747
When N = 10, En/e0 =  1.0604497934468193
When N = 20, En/e0 =  1.0603621577401106
When N = 50, En/e0 =  1.0603620904842708
```

In [13]:
```
plt.figure(dpi=100)
plt.scatter(index1, eigenValues1, label = 'N=1')
plt.plot(index2, eigenValues2, label = 'N=2')
plt.plot(index5, eigenValues5, label = 'N=5')
plt.plot(index10, eigenValues10, label = 'N=10')
plt.plot(index20, eigenValues20, label = 'N=20')
plt.plot(index50, eigenValues50, label = 'N=50')
plt.legend()
plt.grid()
plt.ylabel(r'Exact energy with unit $\left(\frac{\hbar^{2}}{2 m_{0}}\right)^{2 / 3} \lambda^{1 / 3}$')
plt.xlabel(r'$n$')
```

Out[13]: Text(0.5,0,'n')



The the deviations are truncation error, now zoom N from 0 to 20

In [14]:
```
plt.figure(dpi=100)
plt.scatter(index1, eigenValues1, label = 'N=1')
plt.plot(index2, eigenValues2, label = 'N=2')
plt.plot(index5, eigenValues5, label = 'N=5')
plt.plot(index10, eigenValues10, label = 'N=10')
plt.plot(index20, eigenValues20, label = 'N=20')
plt.plot(index50, eigenValues50, label = 'N=50')
plt.xlim(-0.25, 20)
plt.ylim(-10, 500)
plt.legend()
plt.grid()
plt.ylabel(r'Exact energy with unit $\left(\frac{\hbar^{2}}{2 m_{0}}\right)^{2 / 3} \lambda^{1 / 3}$')
plt.xlabel(r'$n$')
```

Out[14]:
```
Text(0.5,0,'$n$')
```