Q1 numerical

For $V_0 = 0$

$$H_{nm} = \langle \psi_n | (H_0 + V) | \psi_m \rangle = \delta_{nm} E_n^{(0)} + \frac{2V_1}{a} \int_{a/2}^{a} dx \sin\Big(\frac{n\pi x}{a}\Big) \sin\Big(\frac{m\pi x}{a}\Big)$$

Which is solve as[1]:

$$\begin{aligned} h_{nm} \equiv & H_{nm}/E_1^{(0)} \\ = & \delta_{nm} \left[n^2 + v_0 \left(\frac{1}{2} - \frac{\sin 2\pi n - \sin \pi n}{2\pi n} \right) \right] \\ & + v_0 \left(1 - \delta_{nm}\right) \left(\frac{\sin(n-m)\pi - \sin(n-m)\frac{\pi}{2}}{\pi(n-m)} - \frac{\sin(n+m)\pi - \sin(n+m)\frac{\pi}{2}}{\pi(n+m)} \right) \end{aligned}$$

[1]Marsiglio, F., 2009. The harmonic oscillator in quantum mechanics: A third way. American Journal of Physics, 77(3), pp.253-258.

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

In [3]:
```
rho = 1/2
rho1 = 1
rho0 = 1/2
def delta(n, m):
    if m==n:
        return 1
    else:
        return 0

def term1(n, m, v0):
    func = rho - (np.sin(2*np.pi*n*rho1)-np.sin(2*np.pi*n*rho0))/(2*np.pi*n)
    return delta(n, m)*(n**2+v0*func)


def term2(n, m, v0):
    if n == m:
        return 0
    else:
        func = (np.sin((n-m)*np.pi*rho1)-np.sin((n-m)*np.pi*rho0))/(np.pi*(n-m))-(np.si
n((n+m)*np.pi*rho1)-np.sin((n+m)*np.pi*rho0))/(np.pi*(n+m))
        return v0*(1-delta(n, m))* func
```

In [4]:
```
size = 500
v0 = 4000
i = 0

hij = np.zeros((size, size))
while i<size:
    j = 0
    while j<size:
        hij[i, j] = term1(i+1, j+1, v0) + term2(i+1, j+1, v0)
        j = j+1
    i = i+1

eigenValues, eigenVectors = la.eig(hij)
eigenValues = np.real(eigenValues)
index = np.linspace(1, size, size)

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

For $E > V_1$

$$E_n/E_1^{(0)} = \frac{E_n^{(0)}}{2E_1^{(0)}} + \frac{V_1}{2E_1^{(0)}} + \frac{V_1^2}{16E_n^{(0)}E_1^{(0)}} = n^2 + v_1/2 + \frac{v_1^2}{16n^2}$$

For $E < V_1$

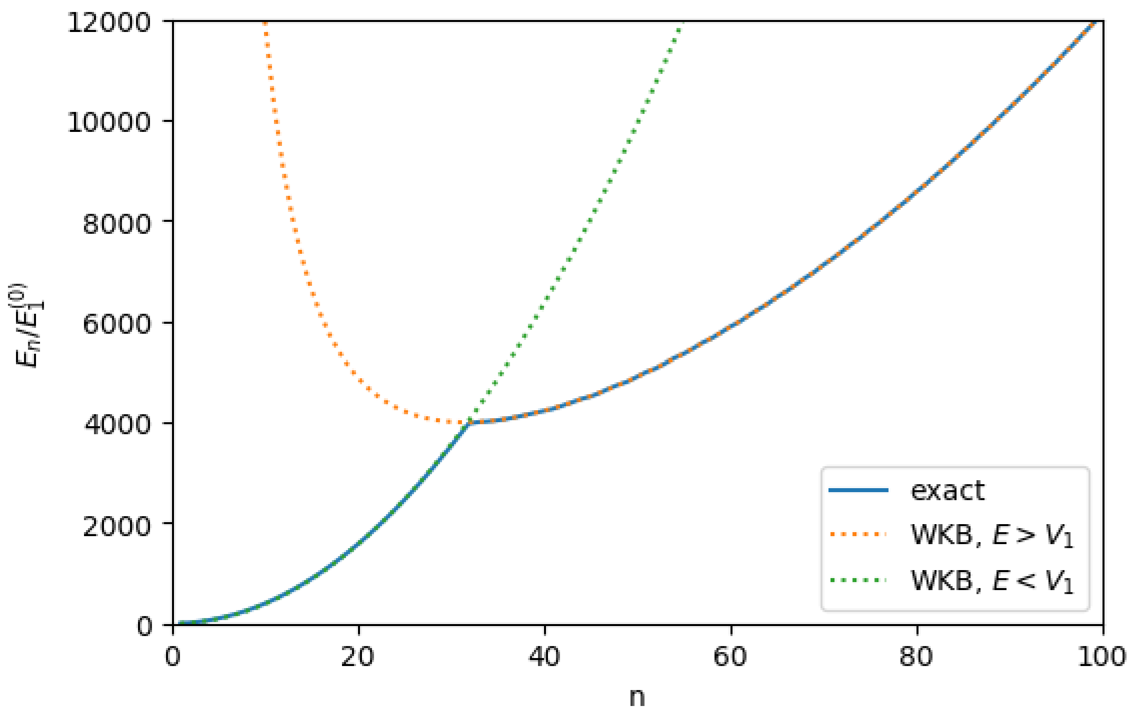
$$E_n/E_1^{(0)} = 4n^2 - 2n + 1/4$$

Where v_1 is $V_1/E_1^{(0)}$ for $E_1^{(0)}$ is ISW ground state energy.

In [5]:
```
e0 = index**2+v0/2+v0**2/(16*index**2)
e0_sm = 4*index**2-2*index+1/4
```

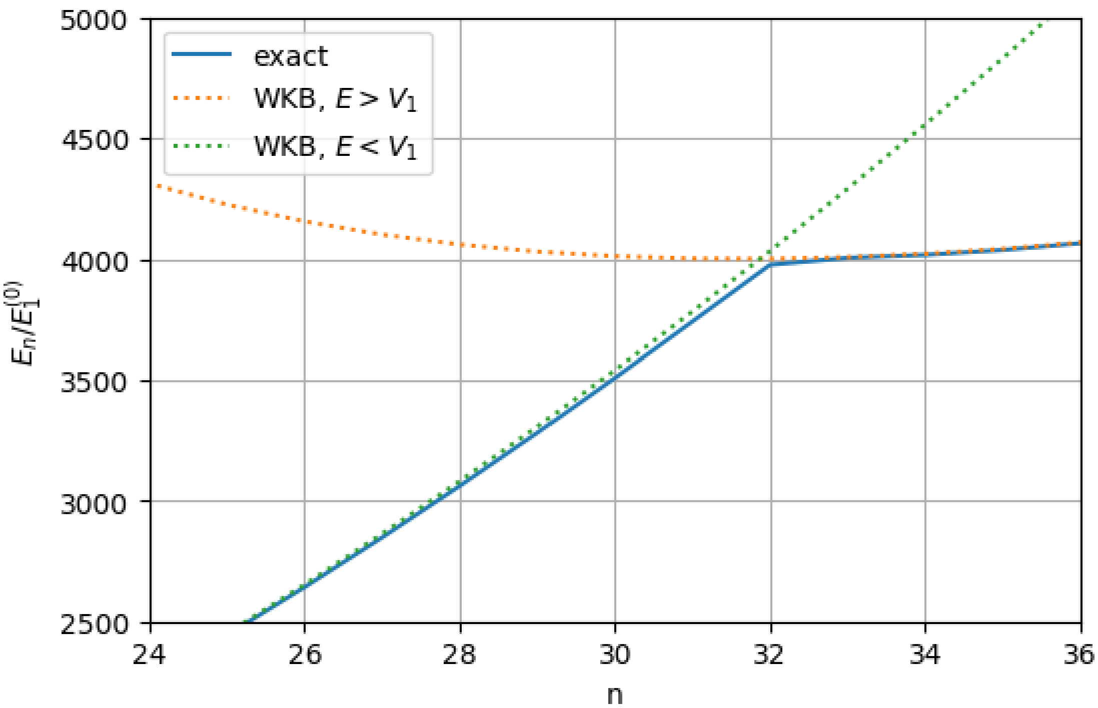
In [17]:
```
plt.figure(dpi=100)
plt.plot(index, eigenValues, label = 'exact')
plt.plot(index, e0, label = r'WKB, $E>V_1$', linestyle = 'dotted')
plt.plot(index, e0_sm, label = r'WKB, $E<V_1$', linestyle = 'dotted')
plt.xlim(0,100)
plt.ylim(0, 12000)
plt.ylabel(r'$E_n/E_1^{(0)}$')
plt.xlabel('n')
plt.legend()
```

Out[17]: <matplotlib.legend.Legend at 0x7f449a321898>



The result almost overlapping, now zoom in.

In [15]:
```
plt.figure(dpi=100)
plt.plot(index, eigenValues, label = 'exact')
plt.plot(index, e0, label = r'WKB, $E>V_1$', linestyle = 'dotted')
plt.plot(index, e0_sm, label = r'WKB, $E<V_1$', linestyle = 'dotted')
plt.xlim(24,36)
plt.ylim(2500, 5000)
plt.ylabel(r'$E_n/E_1^{(0)}$')
plt.xlabel('n')
plt.legend()
plt.grid()
```



Q2. c) Compare

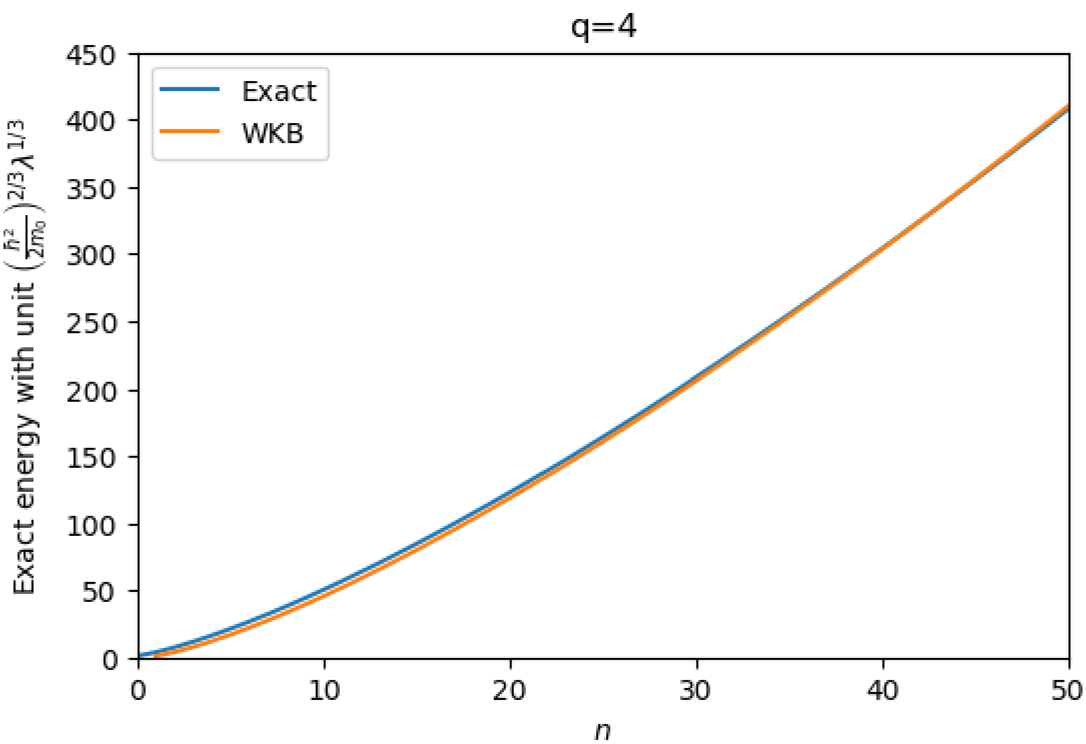
By using the code from assignment 8 calculate the energy for q=4.

In [81]:
```
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-1, size)

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

    return eigenValues, eigenVectors, index

es10, evs10, ns10 = isw(10, 1000)
```

In [133]:
```
e4 = 1.113*3/(8)*np.pi**(2/3)*(2*ns10-1)**(4/3)

plt.figure(dpi=100)
plt.plot(ns10, es10/10**2, label = 'Exact')
plt.plot(ns10, e4, label = 'WKB')
plt.xlim(0, 50)
plt.ylim(0, 450)
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.title('q=4')
plt.legend()
```

```
/home/alex/.local/lib/python3.6/site-packages/ipykernel_launcher.py:1: RuntimeWarning: invalid value encountered in power
  """Entry point for launching an IPython kernel.
```

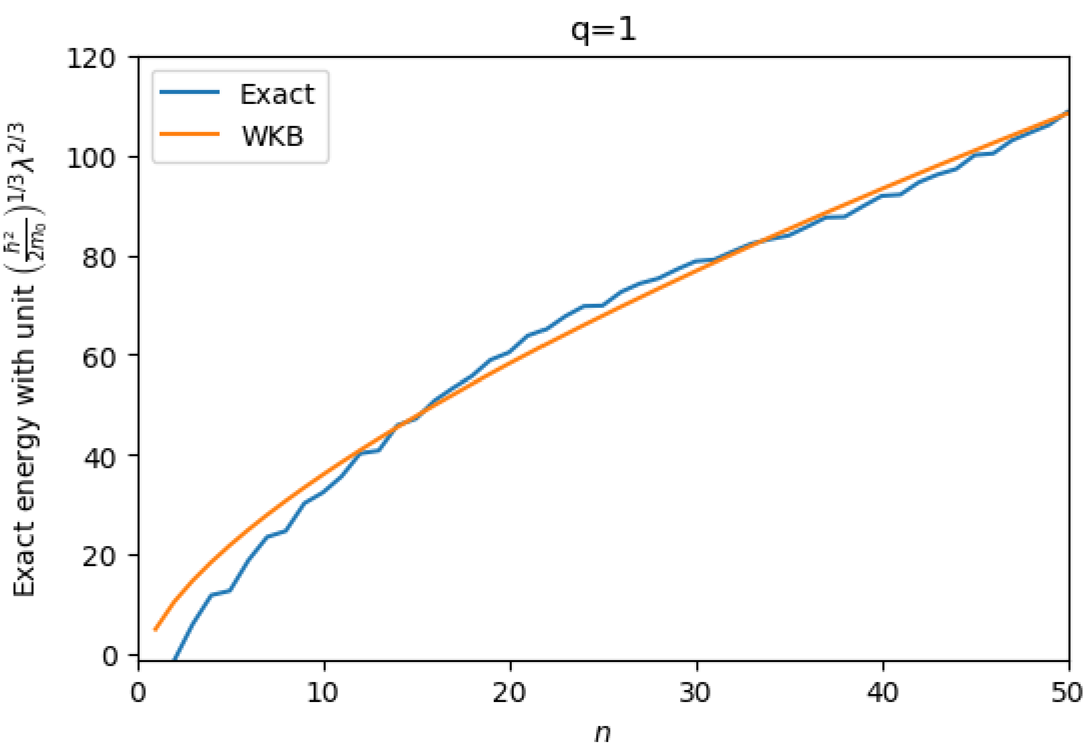
Out[133]: <matplotlib.legend.Legend at 0x7f4495470fd0>



In [124]:
```
def vij(m, n):
    if m==n:
        return 1 / 4 * ( 1- (4 / (np.pi*n) ** 2 * (1-(-1)**n)/2) )
    else:
        return 4 / np.pi**2 * ( (1+(-1)**(n+m)) /2) * ( (1-(-1)**((n-m))/2) / (n-m)**2
- (1-(-1)**((n+m)/2))/(n-m)**2)

def iswq1(lal, 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) + lal*vij(i+1, j+1)
            elem = np.real(elem)
            hij[i, j] = elem
            j = j+1
        i = i+1

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

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

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

    return eigenValues, eigenVectors, index

es1, evs1, ns1 = iswq1(15000, 1000)
```

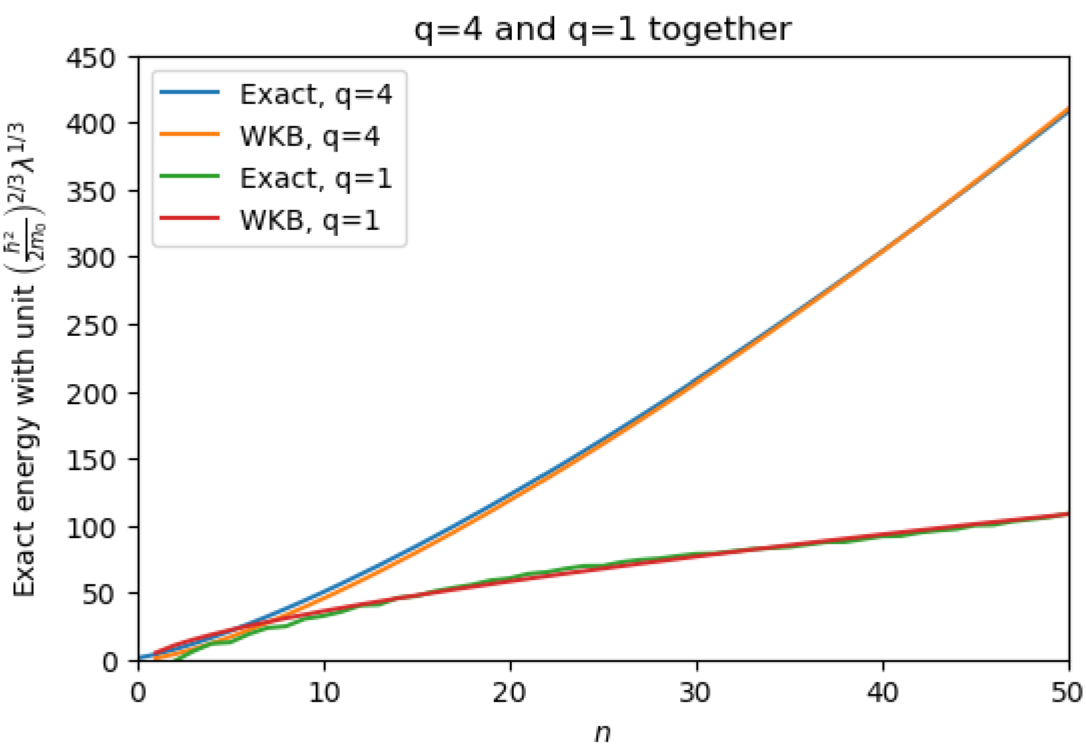
In [137]:
```
e1 = (np.pi*8/3)*3**(2/3)/2*np.pi**(1/3)*(ns1-1/2)**(2/3)/2**(2/3)
plt.figure(dpi=100)
plt.plot(ns1, 2*es1/np.sqrt(15000), label = 'Exact')
plt.plot(ns1, e1, label = 'WKB')
#plt.plot(ns10, e4, label = 'WKB')
plt.xlim(0, 50)
plt.ylim(-1, 120)
plt.ylabel(r'Exact energy with unit $\left(\frac{\hbar^{2}}{2 m_{0}}\right)^{1 / 3} \lambda^{2/ 3}$')
plt.xlabel(r'$n$')
plt.title('q=1')
plt.legend()
```

Out[137]: <matplotlib.legend.Legend at 0x7f44951fde10>



In [135]:
```
plt.figure(dpi=100)
plt.plot(ns10, es10/10**2, label = 'Exact, q=4')
plt.plot(ns10, e4, label = 'WKB, q=4')
plt.plot(ns1, 2*es1/np.sqrt(15000), label = 'Exact, q=1')
plt.plot(ns1, e1, label = 'WKB, q=1')
plt.xlim(0, 50)
plt.ylim(0, 450)
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.title('q=4 and q=1 together')
plt.legend()
```

Out[135]: <matplotlib.legend.Legend at 0x7f4495354b70>



In [ ]: