Partition_Functions

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[1]:
```python
__author__ = "Tomás Sánchez Sánchez-Pastor"
__date__   = "06/10/2021"
import numpy as np
from numpy import pi
import matplotlib.pyplot as plt
plt.rc('text',usetex=True)
plt.rc('font',family='serif')
ref_ticksize = 16
plt.rcParams['xtick.labelsize']=ref_ticksize
plt.rcParams['legend.fontsize']=ref_ticksize
plt.rcParams['ytick.labelsize']=ref_ticksize
plt.rcParams['axes.labelsize']=ref_ticksize * 3/2
plt.rcParams['axes.titlesize']=ref_ticksize * 3/2
```

The quantum partition function of a system with eigenergies ε_ν is computed as

$$Z = \sum_{\nu=0}^{\infty} e^{-\beta\varepsilon_\nu},$$

with $\beta = \frac{1}{k_B T}$, being k_B the Boltzmann's constant. It is closely related with the probability distribution of N particles in the system

$$P(\nu) = \frac{1}{Z} e^{-\beta\varepsilon_\nu}$$

0.1 Harmonic Oscillator

$$\varepsilon_\nu = \hbar\omega(\nu + 1/2)$$

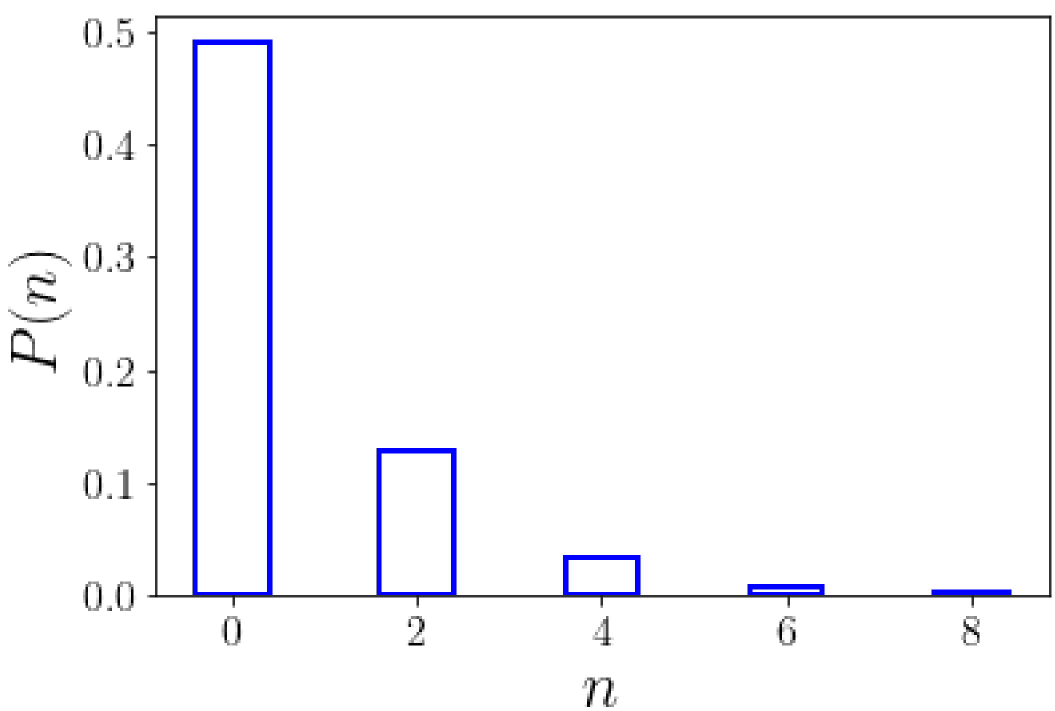
[59]:
```python
kb   = 1.38064852e-23  # J/K
T    = 1e-9            # K
beta = 1/(kb*T)        # 1/J
hbar = 1.054571817e-34 # J·s
w    = 2*np.pi*14      # rad/s
n    = np.arange(0, 10, 2)
```

[60]:
```python
def eho(nu):
    return hbar*w*(nu+1/2)
```

[61]:
```
Zho = np.exp(-beta*hbar*w/2) / (1 - np.exp(-beta*hbar*w))
Pho = 1/Zho * np.exp(-beta*eho(n))
```

[62]:
```
fig, ax = plt.subplots()
ax.bar(n, Pho, edgecolor='b', facecolor='w', lw=2)
ax.set_xlabel(r'$n$')
ax.set_ylabel(r'$P(n)$')
print(f'''
--------------------
n             P(n)
--------------------
0            {round(Pho[0]*100, 2)}%
2            {round(Pho[1]*100, 2)}%
4            {round(Pho[2]*100, 2)}%
6            {round(Pho[3]*100, 2)}%
8            {round(Pho[4]*100, 2)}%''')
```

```
--------------------
n             P(n)
--------------------
0            48.93%
2            12.76%
4            3.33%
6            0.87%
8            0.23%
```



0.2 Anharmonic Oscillator (sextic)

$$\varepsilon_\nu = \hbar\omega(\nu + 1/2) - \frac{\hbar^2\omega^2}{16V}(\nu^2 + \nu + 1/2) + \frac{\hbar^3\omega^3}{1152V}(4\nu^3 + 6\nu^2 + 8\nu + 3)$$

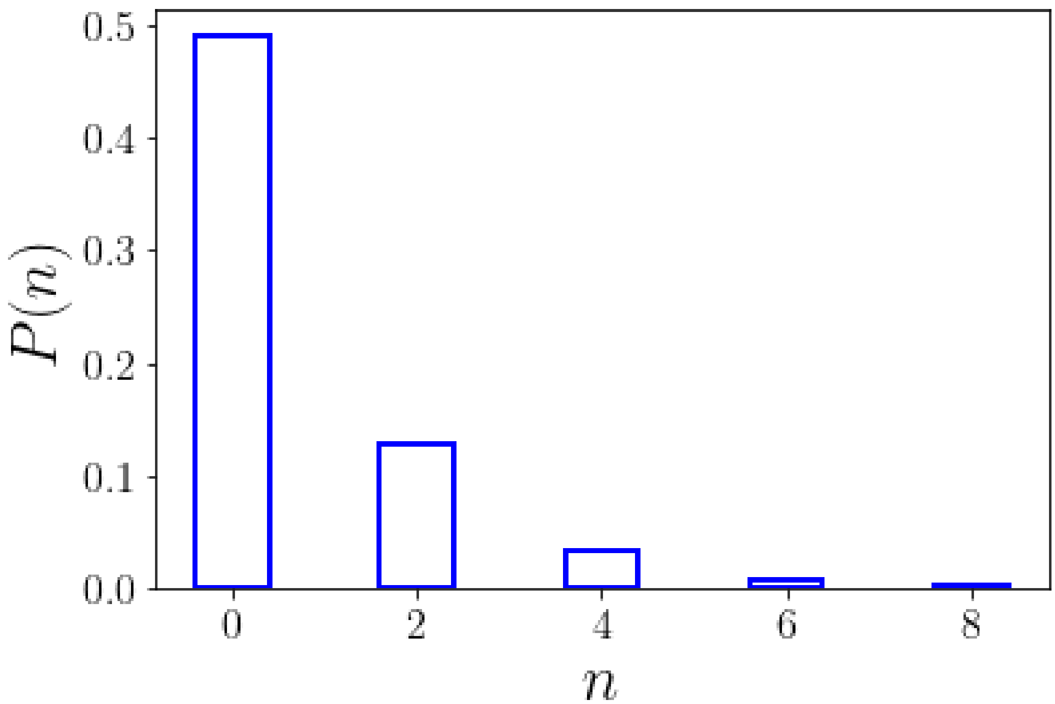
[63]:
```
V = 1.5514861655061523e-10/6.436409310e15
```

[64]:
```
def eah(nu):
    return hbar*w*(nu+1/2) - hbar**2*w**2/(16*V)*(nu**2+nu+1/2) + hbar**3*w**3/
↪(1152*V)*(4*nu**3 + 6*nu**2 + 8*nu + 3)
```

[65]:
```
Zah = 0
for i in range(20):
    Zah += np.exp(-beta*eah(i))
Pah = 1/Zah * np.exp(-beta*eah(n))
```

[66]:
```
fig, ax = plt.subplots()
ax.bar(n, Pah, edgecolor='b', facecolor='w', lw=2)
ax.set_xlabel(r'$n$')
ax.set_ylabel(r'$P(n)$')
print(f'''
--------------------
n              P(n)
--------------------
0             {round(Pho[0]*100, 2)}%
2             {round(Pho[1]*100, 2)}%
4             {round(Pho[2]*100, 2)}%
6             {round(Pho[3]*100, 2)}%
8             {round(Pho[4]*100, 2)}%''')
```

```
--------------------
n              P(n)
--------------------
0             48.93%
2             12.76%
4             3.33%
6             0.87%
8             0.23%
```



Conclusion: The anharmonic correction can be neglected when measuring the level probability distribution