In [4]:
```python
import pandas as pd
import numpy as np
import matplotlib.pyplot as plt
```

Exercise 2

In [2]:
```python
N = np.arange(200, 1200, 200)
```

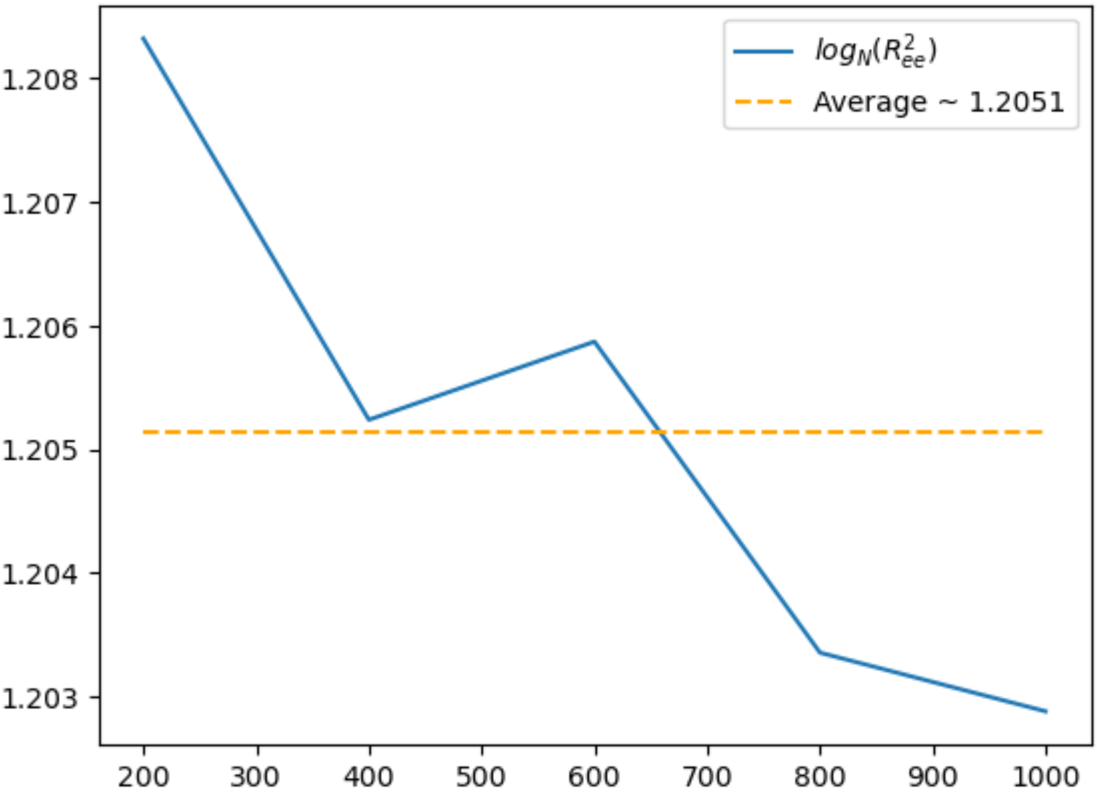
In [3]:
```python
dfs = {}
for i in N:
    dfs[i] = pd.read_csv(f'analysis/analysis%d' % i, sep=' ', header=None)
```

In [4]:
```python
R2ee = {}
for i in N:
    R2ee[i] = np.mean(dfs[i][1])
R2ee = np.array(list(R2ee.values()))
```

In [5]:
```python
# plt.plot(N, R2ee)
plt.plot(N, np.emath.logn(N, R2ee), label='$log_N(R^2_{ee})$')
meanlog = np.mean(np.emath.logn(N, R2ee))
print(meanlog)
plt.hlines(meanlog, N[0], N[-1], linestyles='dashed', color='orange', label='Average ~ 1.2051'
plt.legend()
```

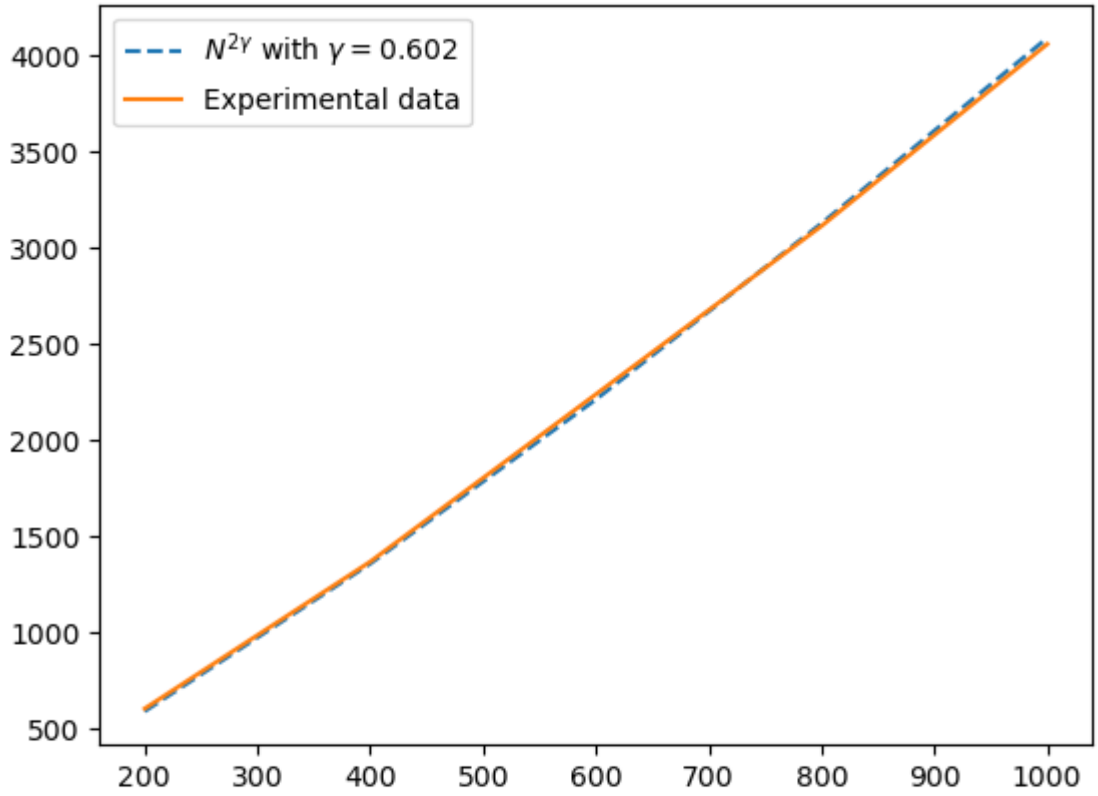
```
1.205132636171456
```

Out[5]: `<matplotlib.legend.Legend at 0x7faa451ea860>`



In [6]:
```python
plt.plot(N, N**1.204, '--', label='$N^{2 \gamma}$ with $\gamma = 0.602$')
plt.plot(N, R2ee, label='Experimental data')
plt.legend()
```

Out[6]: `<matplotlib.legend.Legend at 0x7faa3c6c7a90>`



Exercise 3

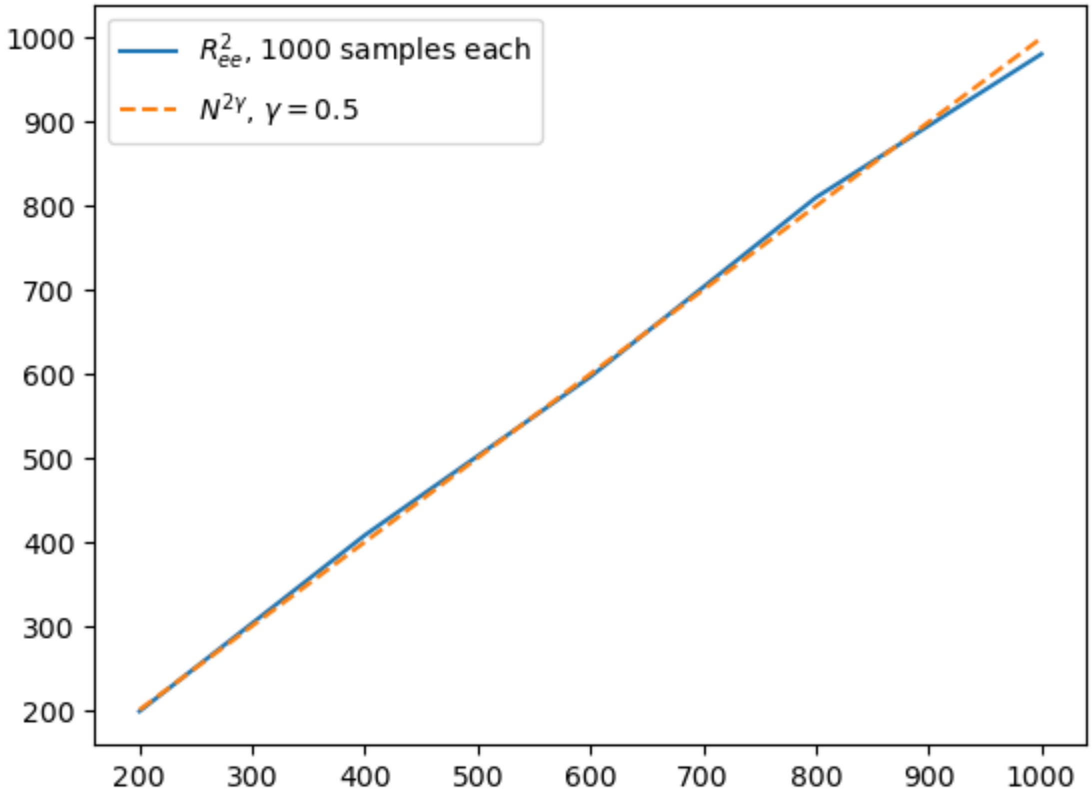
In [5]:
```
def sample_R2ee(N, samples = 1000):
    μ = 0.0 # Average end to end radius
    r = np.array([[-1 , 0], [1, 0], [0, 1], [0, -1]]) # directions
    for _ in range(samples):
        # generate 'samples' random walks, calculate R2ee and calculate average
        walk = r[np.random.randint(0, 4, N)] # generates a random walk with N steps
        R = walk.sum(axis=0)
        μ += np.dot(R, R) / samples
    return μ
```

In [6]:
```
%%time
N = np.array([200, 400, 600, 800, 1000])
R2ee = np.array([sample_R2ee(N) for N in N])
```

```
CPU times: user 368 ms, sys: 2.86 ms, total: 370 ms
Wall time: 369 ms
```

In [7]:
```
plt.plot(N, R2ee, label='$R^2_{ee}$, 1000 samples each')
plt.plot(N, N, '--', label='$N^{2 \gamma}$, $\gamma = 0.5$')
plt.legend()
```

Out[7]:
```
<matplotlib.legend.Legend at 0x7fef4064b0d0>
```

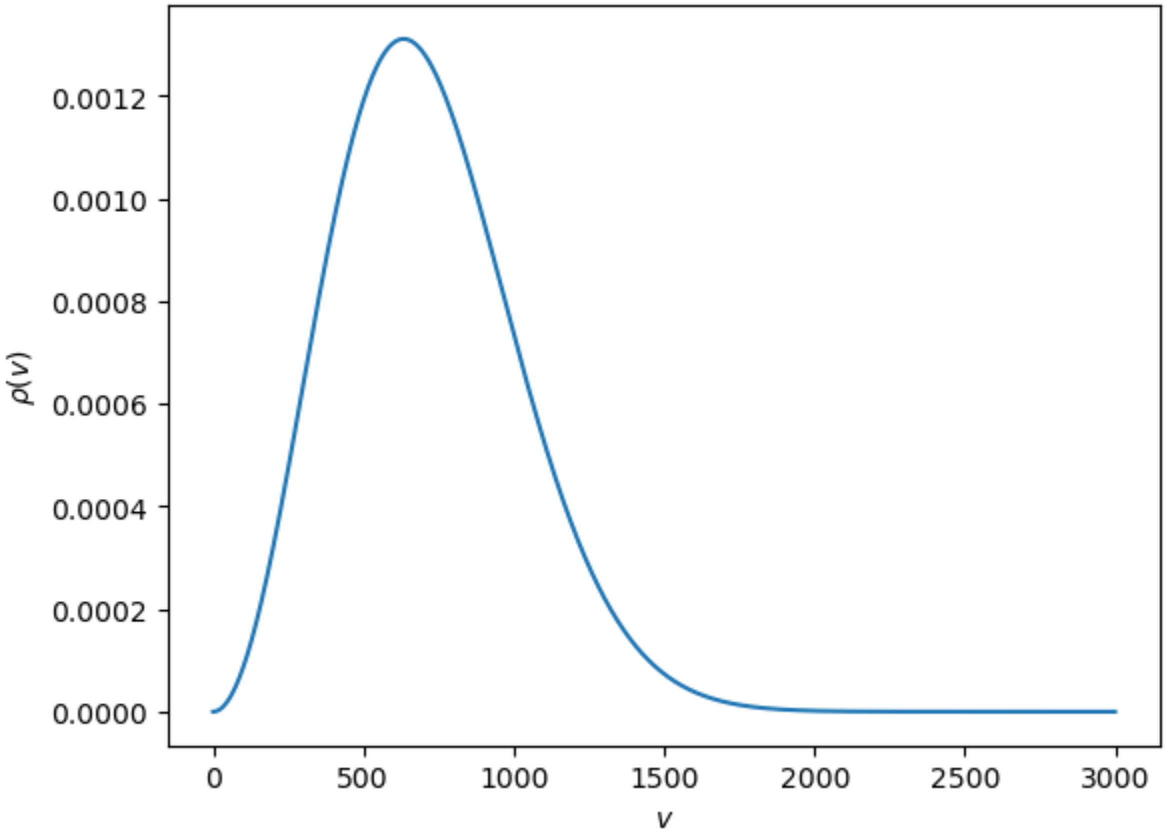


Exercise 4

In [7]:
```
from scipy.constants import k, pi, N_A, h
```

In [8]:
```
M = 60.08e-3 # kg/mol
m = M / N_A
T = 1450
v = np.arange(0, 3e3)
rho = (m / (2*pi*k*T))**1.5 * 4*pi*v*v*np.exp(-m*v*v/(2*k*T))
```

In [21]:
```
plt.plot(v, rho)
plt.xlabel('$v$')
plt.ylabel('$\\rho(v)$')
plt.show()
```


0.0012
0.0010
0.0008
0.0006
0.0004
0.0002
0.0000
$\rho(v)$
0
500
1000
1500
2000
2500
3000
v

b)

Given: $\rho(v) = 4\pi\left(\frac{c}{2\pi}\right)^{\frac{3}{2}} v^2 e^{-\frac{cv^2}{2}}$, with $c = \frac{m}{k_B T}$, calculate $\langle v\rangle = \int_0^\infty v\rho(v)\,\mathrm{d}x$.

$$\Rightarrow \langle v\rangle = \int_0^\infty v\rho(v)\,\mathrm{d}x \tag{1}$$
$$= \int_0^\infty 4\pi\left(\frac{c}{2\pi}\right)^{\frac{3}{2}} f(v)g(v)\,\mathrm{d}x \tag{2}$$
$$= 4\pi\left(\frac{c}{2\pi}\right)^{\frac{3}{2}} \int_0^\infty f(v)g(v)\,\mathrm{d}x \tag{3}$$
$$= 4\pi\left(\frac{c}{2\pi}\right)^{\frac{3}{2}} \left([f(v)G(v)]_0^\infty - \int_0^\infty 2vG(v)\,\mathrm{d}x\right) \tag{4}$$
$$= 4\pi\left(\frac{c}{2\pi}\right)^{\frac{3}{2}} \left(\underbrace{\left[-v^2\frac{e^{-\frac{cv^2}{2}}}{c}\right]_0^\infty}_{\to 0} + \frac{2}{c}\int_0^\infty v^2 e^{-\frac{cv^2}{2}}\,\mathrm{d}x\right) \tag{5}$$
$$= 4\pi\left(\frac{c}{2\pi}\right)^{\frac{3}{2}} \frac{2}{c}\int_0^\infty vg(v)\,\mathrm{d}x \tag{6}$$
$$= 4\pi\left(\frac{c}{2\pi}\right)^{\frac{3}{2}} \frac{2}{c}\left(\underbrace{\left[-v\frac{e^{-\frac{cv^2}{2}}}{c}\right]_0^\infty}_{\to 0} + \frac{1}{c}\underbrace{\int_0^\infty e^{-\frac{cv^2}{2}}}_{=1}\right) \tag{7}$$
$$= 4\pi\left(\frac{c}{2\pi}\right)^{\frac{3}{2}} \frac{2}{c^2} \tag{8}$$
$$= 2\frac{\pi}{\pi^{\frac{3}{2}}}\frac{\left(\frac{c}{2}\right)^{\frac{3}{2}}}{\left(\frac{c}{2}\right)^2} \tag{9}$$
$$= \sqrt{\frac{8}{c\pi}} \tag{10}$$

c)

$$\langle p\rangle = m\langle v\rangle = m\sqrt{\frac{8k_BT}{\pi m}} = \sqrt{\frac{8mk_BT}{\pi}} = \frac{2}{\pi}\sqrt{2\pi m k_B T} = \frac{2}{\pi}p_T \tag{11}$$
$$\Rightarrow \lambda = \frac{\pi}{2}\lambda_T \tag{12}$$

d)

In [23]:
```
wl = pi / 2 * h / np.sqrt(2 * pi * m * k * T) # m
bl = 1.6e-10 # m
print(f"The De Broglie wavelength of SiO2 is ~%d%% of the bond length. Therefore we ignore qua
```

```
The De Broglie wavelength of SiO2 is ~5% of the bond length. Therefore we ignore quantum effect
s.
```