Question 3. In a random-walk 1D diffusion, use a Gaussian function $exp(\frac{\delta x^2}{\sigma^2})$ to determine step size δx.Find the temperature of analytic result that best fits the random-walk diffusion.

In [1]:

```
import numpy as np
import matplotlib.pyplot as plt
import random
```

In [2]:

```
# Number of particles to use for simulation
N = int(10000)

# Size of the unit walk step.
dx = float(0.1)

# Max steps of simulation
smax = int(110)

# Number of bins for density distribution plot
nBin = 10

# Calculation of theoretical parameters
D = 0.5 * (dx) ** 2  # suppose dt=1
tau = 1.0 / (D * np.pi * np.pi)
```

In [3]:

```
x = np.zeros(N)  # Zero-initialized particle positions
```

In [4]:

```
# Construct the initial sine-distribution of 10000 particles
i = 0
while i < N:
    V = random.random()
    T = random.random()
    val = np.sin(np.pi * V)
    if T <= val:
        x[i] = V
        i += 1
```

In [5]:

```
# Create bin meshes for density distribution
f = np.zeros(nBin + 1)
bnX = np.arange(0, nBin + 1)
bnX = bnX / (1.0 * nBin)  # x-value for the distr-plot
```

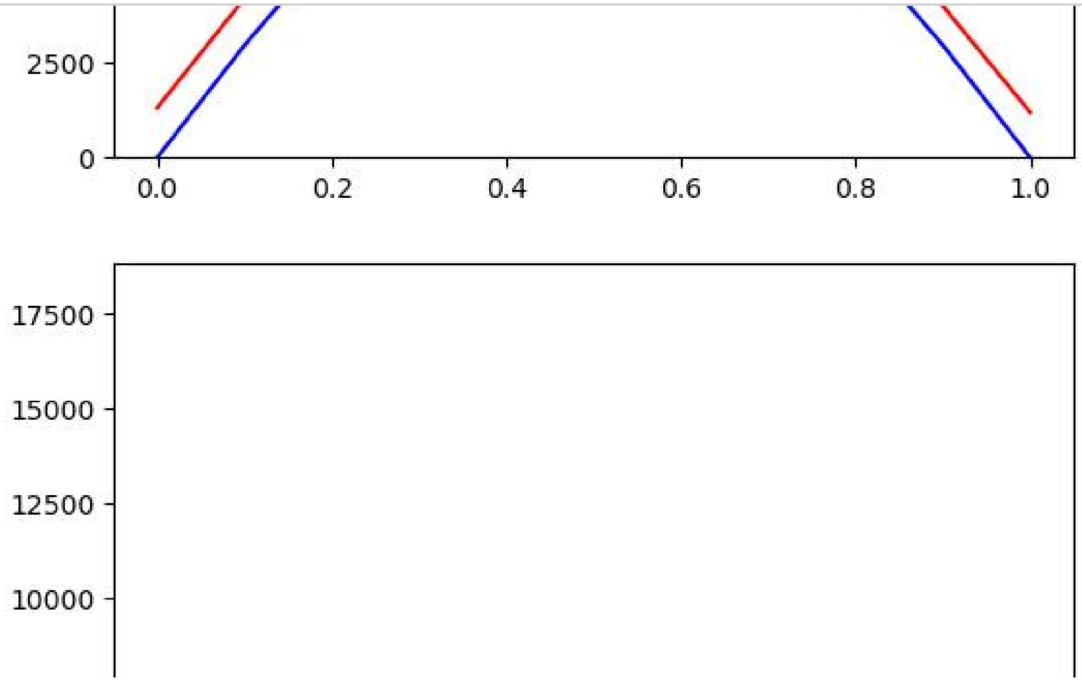
In [6]:

```
#standard deviation
sigma = float(input("Standard deviatioin"))
```

Standard deviatioin0.1

In [7]:

```
# Main loop
for s in range(smax):
    f = 0.0 * f  # empty the bin for new constructon of the distr. every step
    for i in range(N):
        if 0 <= x[i] and x[i] <= 1:
            y = x[i] * (1.0 * nBin)  # normalize the potision to bin
            m = int(y)  # find the bin index
            y -= m  # find the relative displacement in bin
            f[m] += (1.0 - y);
            f[m + 1] += y
            #x[i] = x[i] + random.choice([dx, -dx])
            x[i] = x[i] + np.random.normal(0,sigma,1)[0]  # random walk
    f = (1.0 * nBin) * f  # normalization factor for distri.
    plt.ylim(0, 1.2 * np.pi * N / 2.0)
    z = 0.5 * np.pi * N * np.sin(np.pi * bnX) * np.exp(-(1.0 * s) / tau)
    if s %10 == 0:
        plt.plot(bnX, f, c='r')
        plt.plot(bnX, z, c='b')
        plt.draw()
        plt.pause(0.01)
        plt.clf()
```



When standard deviation is 0.1, it was the best fit.

What is the relation between σ and the temperature? Can you explain it physically?

Maxwell-Boltzman speed distribution in 1 dimension is $g(v_x) = \sqrt{\frac{m}{2\pi k_B T}} e^{\frac{-mv^2}{2k_B T}}$.

That is, $\sigma = \sqrt{\frac{2\pi k_B T}{m}}$

Therefore, σ is proportional to square of T

For each standard deviationi, we can calculate T From $\tau = \frac{1}{\pi^2 D} = \frac{mv}{\pi^2 k_B T}$

In [45]:

```
def scatter_sine(x,N) :
    i = 0
    while i < N:
        V = random.random()
        T = random.random()
        val = np.sin(np.pi * V)
        if T <= val:
            x[i] = V
            i += 1
    return x
```

In [52]:

```
def rwd(smax, N, f, x, sigma) :
    for s in range(smax):
        f = 0.0 * f  # empty the bin for new constructon of the distr. every step
        for i in range(N):
            if 0 <= x[i] and x[i] <= 1:
                y = x[i] * (1.0 * nBin)  # normalize the potision to bin
                m = int(y)  # find the bin index
                y -= m  # find the relative displacement in bin
                f[m] += (1.0 - y);
                f[m + 1] += y
                #x[i] = x[i] + random.choice([dx, -dx])
                x[i] = x[i] + np.random.normal(0,sigma,1)[0]  # random walk
        f = (1.0 * nBin) * f  # normalization factor for distri.

        if s == 0 :
            fsum_0 = np.sum(f)

        if np.sum(f)/fsum_0 <= 1/np.e :
            ct = s
            break


    return ct
```

In [50]:

```
ct = np.zeros(5) # measured characteristic time
T = np.zeros(5) # temperature
st = np.array([0.02,0.04,0.06,0.08,0.1]) # standard deviation
```

In [53]:

```
for i in range(5) :
    x = np.zeros(N)
    sigma = float(i)
    x = scatter_sine(x,N)
    print(st[i])
    ct[i] = rwd(1000, N, f, x, st[i])
    print(ct[i])
    print(1/ct[i])
```

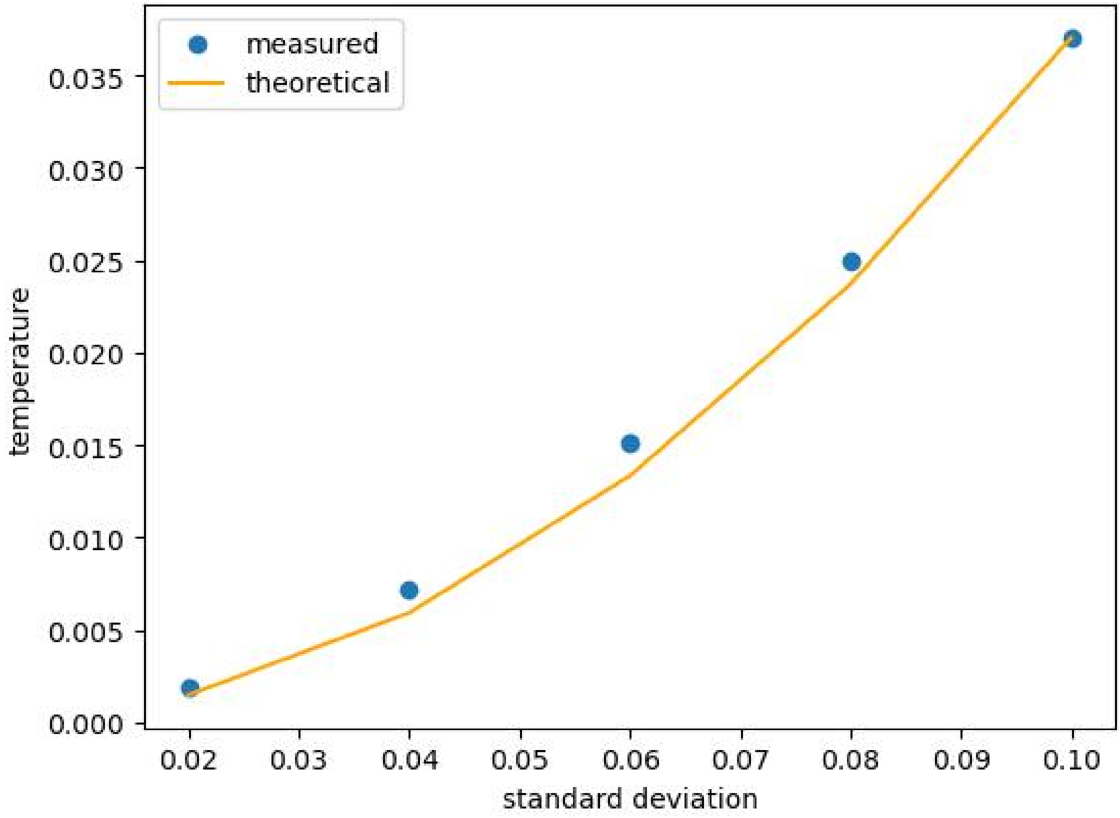
```
0.02
536.0
0.0018656716417910447
0.04
139.0
0.007194244604316547
0.06
66.0
0.015151515151515152
0.08
40.0
0.025
0.1
27.0
0.037037037037037035
```

In [55]:

```
T = 1/ct
```

In [63]:

```
plt.scatter(st,T, label = "measured")
plt.plot(st, (T[4]/st[4]**2)*st**2, label = "theoretical", c = 'orange') #(T[4]/st[4]**2) is coe
plt.xlabel("standard deviation")
plt.ylabel("temperature")
plt.legend()
plt.show()
```



We can see T is proportional to squre of standard deviation