Solution and Discussion for HW problem 9.19

In this problem, we are asked to consider a wavefunction for a 1D particle

$$\psi(x) = \sqrt{\frac{2}{L}} \sin(\frac{2\pi}{L}x),$$

where $L = 10$ nm. You should have recognized that this is a correctly-normalized Particle-in-a-Box (PIB) wavefunction $\psi_n^{PIB}(x)$ for $n = 2$.

The questions asked are:

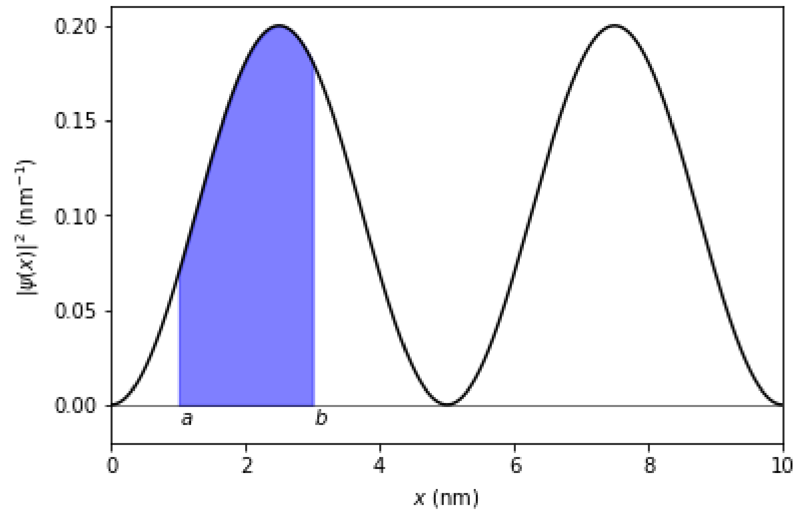
- (a) What is the probability of finding the particle between $x = 0.1$ nm and $x = 0.2$ nm?
- (b) What is the probability of finding the particle between $x = 4.9$ nm and $x = 5.2$ nm?

These are variations on the same calculation,

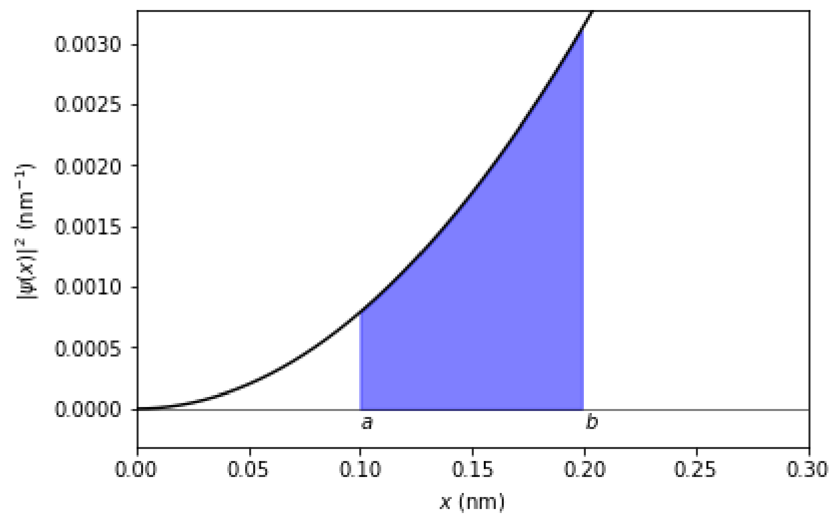
$$\int_a^b P(x)dx = \int_a^b |\psi(x)|^2 dx = \int_a^b \frac{2}{L}\sin^2(\frac{2\pi}{L}x)dx,$$

for different endpoints a and b. We can visualize this as calculating the *area* under the curve $|\psi(x)|^2$ between a and b:

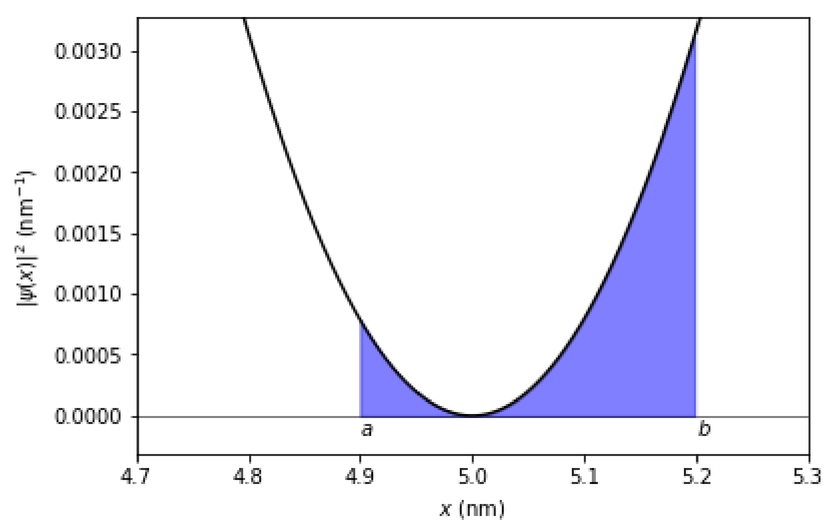
In [12]:
```
import numpy as np
from matplotlib import pyplot as plt
%matplotlib inline

def psi(x, L=10., n=2):
    """Return the value of the nth PIB wavefunction.  x and L are in uni
ts nm."""
    return (2.0/L)**0.5 * np.sin(2.0*np.pi/L*x)


def plot_P(a, b, xrange=[0,10]):

    dx = 0.001 # in nm
    x = np.arange(0, 10.0+dx, dx) #  in nm
    plt.plot(x, (psi(x))**2, 'k-')
    plt.plot([0, 10.0], [0,0], 'k-', linewidth=0.5)

    a_to_b = np.arange(a, b, dx)
    plt.fill_between(a_to_b, psi(a_to_b)*psi(a_to_b), np.zeros(a_to_b.sh
ape), color='b', alpha=0.5)
    plt.xlabel('$x$ (nm)')
    plt.ylabel('$|\psi(x)|^2$ (nm$^{-1}$)')
    plt.xlim(xrange)
    window_max = np.max(psi(a_to_b)*psi(a_to_b))
    plt.ylim(-0.1*window_max, 1.05*window_max)
    plt.text(a, -0.05*window_max, '$a$')
    plt.text(b, -0.05*window_max, '$b$')
    plt.show()

a, b = 1., 3.
plot_P(a,b)

print('For part (a):')
a, b = 0.1, 0.2
plot_P(a, b, xrange=[0,0.3])

print('For part (b):')
a, b = 4.9, 5.2
plot_P(a, b, xrange=[4.7,5.3])
```



For part (a):



For part (b):



How to do the integral

Here's the integral we need to perform: $\int_a^b |\psi(x)|^2 dx = \int_a^b \frac{2}{L}\sin^2(\frac{2\pi}{L}x)dx$

The key formula for the integral (see also: [https://www.wolframalpha.com/calculators/integral-calculator/ (https://www.wolframalpha.com/calculators/integral-calculator/)](https://www.wolframalpha.com/calculators/integral-calculator/)) comes from the trigonometic identity

$\sin^2(x) = \frac{1-\cos(2x)}{2}$.

Therefore,

$\int_a^b \frac{2}{L}\sin^2(\frac{2\pi}{L}x)dx$

$= \frac{2}{L}\left[\int_a^b \frac{1}{2} - \frac{1}{2}\cos(\frac{4\pi}{L}x)dx\right]$

$= \frac{2}{L}\left[\frac{x}{2}\Big|_a^b - \frac{L}{8\pi}\sin(\frac{4\pi}{L}x)\Big|_a^b\right] = \frac{b-a}{L} - \frac{1}{4\pi}\left[\sin(\frac{4\pi}{L}b) - \sin(\frac{4\pi}{L}a)\right]$

In [10]:

```
def evaluate_integral(a, b, L=10.0):
    """Evaluate the integral shown above, and result the result.
    Variables a, b, and L are all in units nm."""

    return (b-a)/L - 1.0/(4.0*np.pi)*( np.sin(4.0*np.pi/L*b) - np.sin(4.
0*np.pi/L*a) )

print('Answer to part (a):')
print( evaluate_integral(0.1, 0.2, 10.0))
print()
print('Answer to part (b):')
print( evaluate_integral(4.9, 5.2, 10.0))
```

```
Answer to part (a):
0.00018358940809886683

Answer to part (b):
0.00023618575264880773
```

Note that the back-of-the-book answer to part (b) is most definitely incorrect. By geometric reasoning (see the plots above!) the answer to (b) must be larger than the answer to (a).