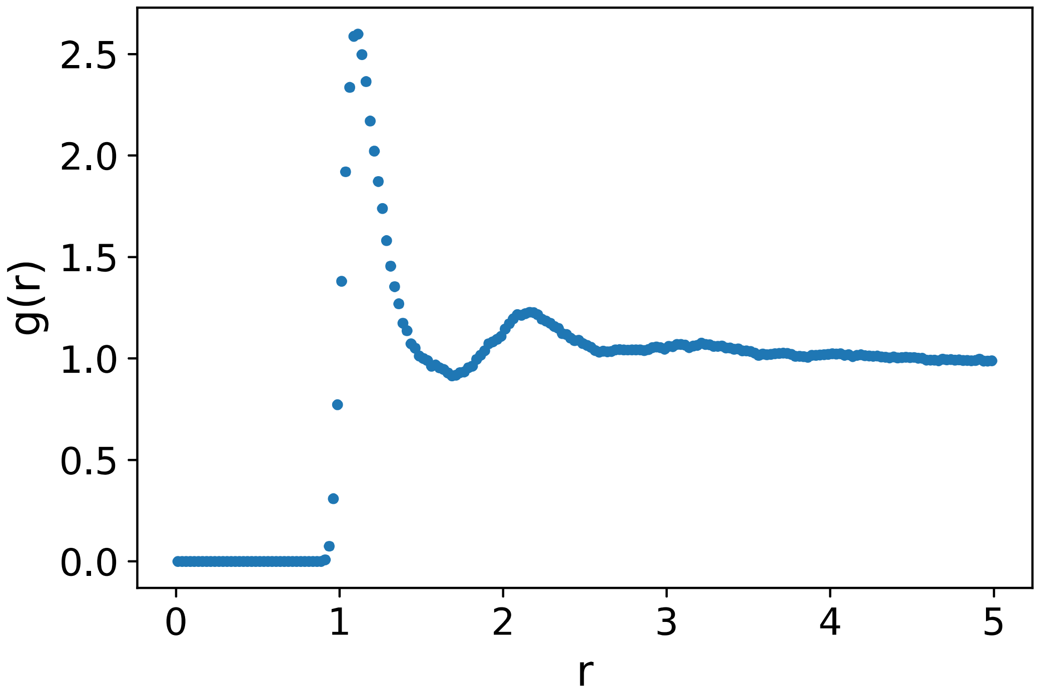
In [2]:
```
import numpy as np
import matplotlib.pyplot as plt
import scipy
import math
```

In [3]:
```
RDF = np.genfromtxt('rdf2.dat',dtype = 'float')
```

In [4]:
```
plt.plot(RDF[:,0],RDF[:,1],'.');
plt.xlabel("r",fontsize = 16);
plt.ylabel("g(r)",fontsize = 16);
plt.xticks(fontsize = 14);
plt.yticks(fontsize = 14);
plt.show()
```



## Calculating structure factor from g(r)

$$\left[S(k) = 1 + 4\pi\rho \int_0^\infty r^2 g(r) \frac{sin(kr)}{kr} dr\right]^*$$

* from Allen and Tildesley

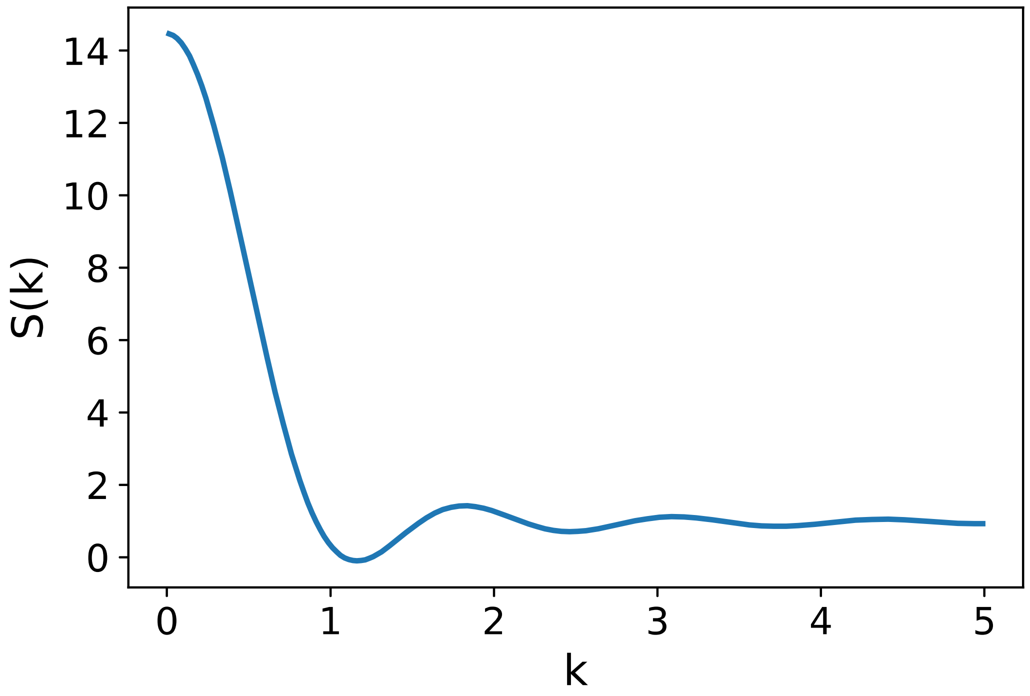
$$\left[S(k) = 1 + 4\pi\rho \int_0^\infty r(g(r)-1) \frac{sin(kr)}{k} dr\right]^+$$

+ A. Filipponi, "The radial distribution function probed by X-ray absorption spectroscopy", Journal of Physics: Condensed Matter 6 pp. 8415-8427 (1994)

In [5]:
```
def Struct_fact1(g_r,r,dr,density):
    S_k = []
    for k in r:
        ind = 0
        integ = 0
        for R in r:
            integ = integ + (R*R*g_r[ind]*(math.sin(k*R)/(k*R))*dr)
            ind = ind + 1
        S_k.append(1 + 4*3.14*density*integ*dr)
    return S_k
def Struct_fact2(g_r,r,dr,density):
    S_k = []
    for k in r:
        ind = 0
        integ = 0
        for R in r:
            integ = integ + (R*(g_r[ind]-1)*(math.sin(k*R)))
            ind = ind + 1
        S_k.append(1 + 4*3.14*density*integ*dr/k)
    return S_k
```

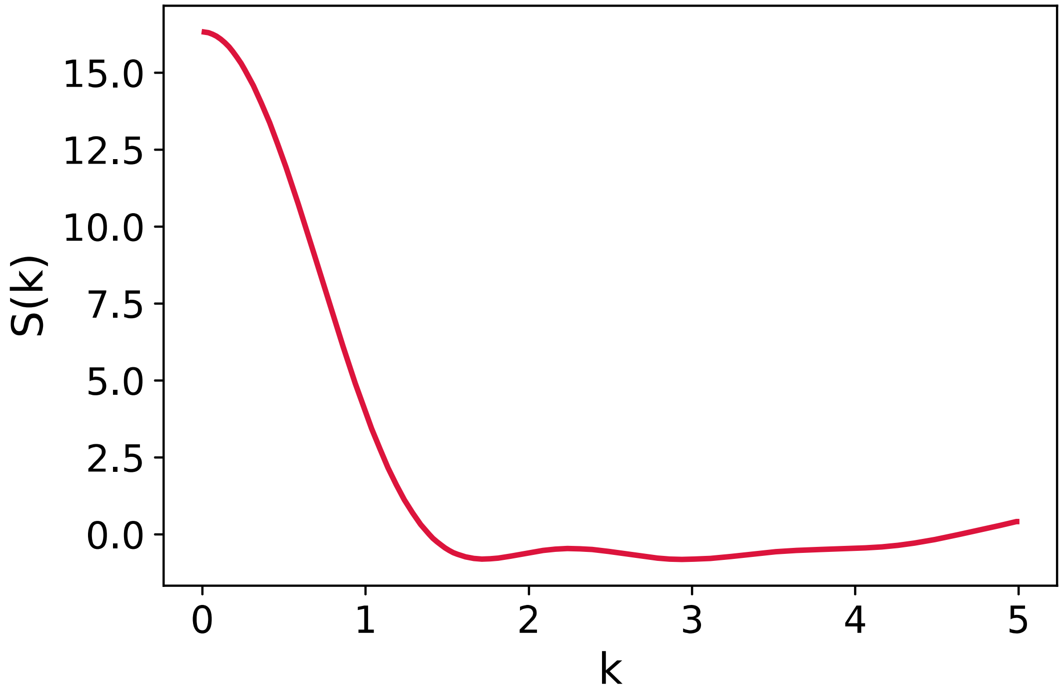
In [6]:

```
dr = RDF[1,0]-RDF[0,0]
density = 1.0
S_k = Struct_fact1(RDF[:,1],RDF[:,0],dr,density)
plt.plot(RDF[:,0],S_k,linewidth = 2);
plt.xlabel("k",fontsize = 16);
plt.ylabel("S(k)",fontsize = 16);
plt.xticks(fontsize = 14);
plt.yticks(fontsize = 14);
plt.show()
```



In [7]:

```
S_k = Struct_fact2(RDF[:,1],RDF[:,0],dr,density)
plt.plot(RDF[:,0],S_k,color = 'crimson',linewidth = 2);
plt.xlabel("k",fontsize = 16);
plt.ylabel("S(k)",fontsize = 16);
plt.xticks(fontsize = 14);
plt.yticks(fontsize = 14);
plt.show()
```

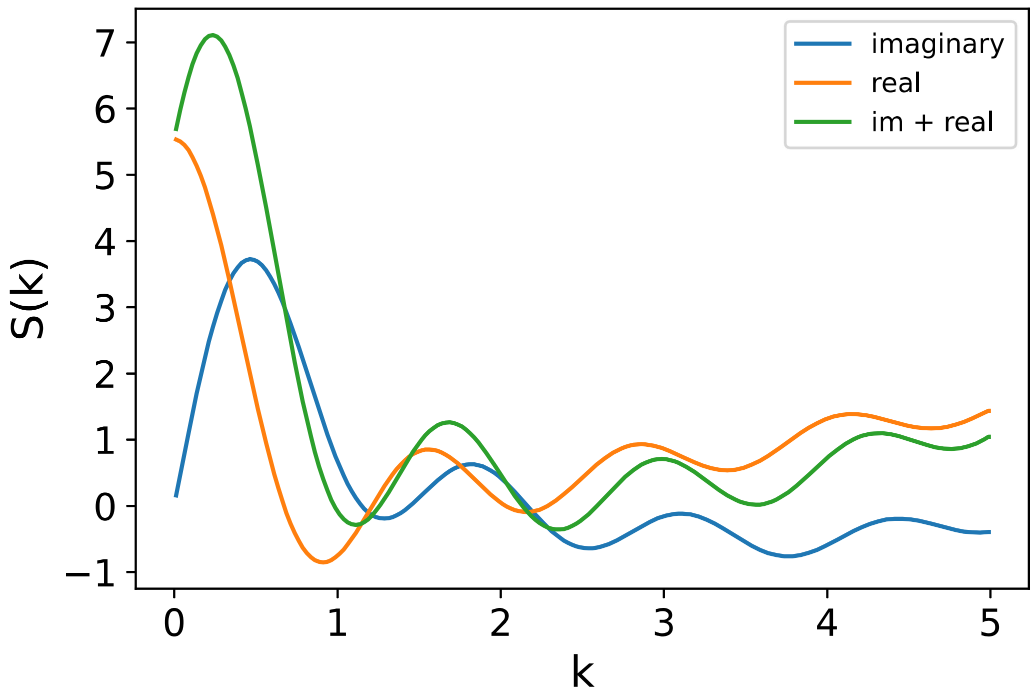


From D.C. Rapaport,

$$S(k) = 1 + \rho \int g(r) e^{-ik.r} dr$$

```
In [33]: import cmath
         r = RDF[:,0]
         k_comp = []
         S_k = []
         g_r = RDF[:,1]
         for k in r:
             ind = 0
             integ = 0
             for R in r:
                 integ = integ + g_r[ind]*cmath.exp(complex(0,(k*R)))*dr
                 ind = ind+1
             S_k.append(1 + density*integ)
```

```
In [47]: S_k = np.array(S_k)
         S_k.real
         plt.plot(r,S_k.imag,label = 'imaginary');
         plt.plot(r,S_k.real,label = "real");
         plt.plot(r,S_k.real+S_k.imag,label = "im + real");
         plt.legend()
         plt.xlabel("k",fontsize = 16);
         plt.ylabel("S(k)",fontsize = 16);
         plt.xticks(fontsize = 14);
         plt.yticks(fontsize = 14);
         plt.show()
```



```
In [ ]:
```