P740.HW2.sol.tex

1. To go from the viscosity to a cross section for a gas at 1 atm and 300 K: $\eta \approx \rho D_\eta$, $D_\eta \approx v\lambda$, $\lambda = 1/n\sigma$ $(\rho = mn)$

$$\sigma \approx \frac{mv}{\eta} \tag{1}$$

where $v^2 \sim k_B T/m$.

When crunching numbers it can help to write a short program

eta.m

```
clear
m=[4 20 40 84 131]';
ep=[10 36 120 170 231]';
sig=[2.56 2.78 3.40 3.64 3.96]';
eta=0.0001*[1.94 3.10 2.21 2.47 2.25]';
rho1=0.00004;
rho=rho1*m;
D=eta./rho;
v1=1.6e5;
v=v1./sqrt(m);
L=D./v;
L8=1.0e8;
Lstar=(L./sig)*L8;
mscale=1.6e-8;
cross16=mscale*m.*v./eta
```

There is a possible ambiguity, the cross section is usually denoted by σ and so is the length scale involved in the Lennard-Jones interaction. But the units are different.

2. Begin with (b). Note that the m in Eq. (3) is in the wrong place. Eq. (2) and (3) are essentially the same. Use

$$\frac{p^2}{2m} - pQ = \frac{1}{2m}(p - mQ)^2 - m\frac{Q^2}{2} = \frac{m}{2}(v-u)^2 - m\frac{Q^2}{2} \tag{2}$$

where $p = mv$ and $u = Q$. Since the p integration is from $-\infty$ to $+\infty$ when calculating the average of p you can shift the origin of integration to $p_Q = mQ$ so that the argument

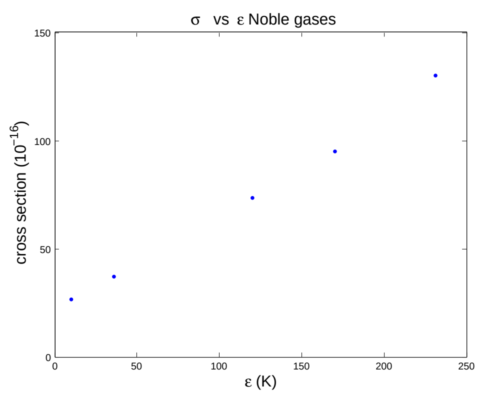

FIG. 1: σ vs ϵ.

in the numerator of the momentum average shifts to mQ, i.e., $p = mQ + (p - mQ)$. Thus $< p >= mQ$. Or using the Eq. (2) above $< p >= mu$.

3. The probability scales as v/v_T where $v_T^2 = 2/m\beta$. So use $x = v/v_T$

$$f(x) = \frac{1}{\sqrt{\pi}} exp(-x^2). \tag{3}$$

Then

$$\int_{-\infty}^{+\infty} dx \ f(x) = 2\int_{0}^{+\infty} dx \ f(x) = 1 \tag{4}$$

and

$$< |v| >= v_T < x >= v_T \ 2\int_{0}^{+\infty} dx \ xf(x) = \frac{v_T}{\sqrt{\pi}}. \tag{5}$$

To find $P_>$ use $x_> = 1/\sqrt{\pi} = 0.5642$ and

$$P_> = 2\int_{x_>}^{+\infty} dx \ f(x) = 1 - 2\int_{0}^{x_>} dx \ f(x) = 1 - erf(x_>) = 0.4249. \tag{6}$$

As a test of the numbers use the cumulative probability, $P(x)$, defined by

$$P(x) = 2\int_{0}^{x} dx \ f(x), \tag{7}$$

the probability that v/v_T is less than x. see Fig. 2. [It doesn't hurt to test results numerically.]

```
% fofv.m
                    clear
% Since f(-x) = f(x) use f(x) = (2/sqrt(pi)) exp - x^2
% values of x, f(x)
                    N=1000;
                    x=linspace(0,6,N)';
                    xx=x.*x;
                    dx=x(2)-x(1);
                    Cnorm=2/sqrt(pi);
                    fofx=Cnorm*exp(-xx);
% dress the norm for numerical errors
                    Inorm=dx*sum(fofx)
                    fofx=fofx/Inorm;
% cumulative probability
                    Pofx=cumsum(dx*fofx);
% < |v| > /v_T
                    vbar=dx*sum(x.*fofx);   % (numerical)
                    vbarT=1/sqrt(pi);   % (analytic)
% compare numerical and analytic result
                    look=[vbar vbarT]
                    Pgreater = 1-erf(vbar)
% to make a figure
                    X=[vbar vbar];
                    Y=[0 1.5];
                    plot(x,fofx,X,Y,x,Pofx)
                    axis([0 3 0 1.2])
                    xlabel('x = v/v_T','Fontsize',16)
                    ylabel('f(x)','Fontsize',16)
                    title('f(x) and P(x) vs x','Fontsize',16)
```

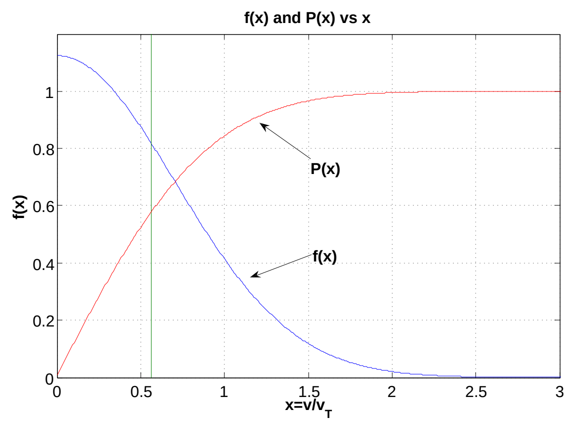

FIG. 2: $f(x)$ and $P(x)$ vs x..

grid

4. This is essentially the same as problem 3 on HW1. For $\epsilon \ll 1$ expect

$$< x > \ = \ \epsilon a N = \epsilon a \frac{t}{\tau}, \tag{8}$$

$$< x^2 > - < x >^2 \ = \ a^2 N = a^2 \frac{t}{\tau}, \tag{9}$$

where a is the step length and τ is the step time. The particles average position moves proportional to time. The particle diffuses relative to its average position just as it does when there is no bias. When ϵ approaches 1 this simple result is modified as it must be for at $\epsilon = 1$ the walk is a completely deterministic walk, every step to the right.