Neutron Interaction Resonances

Table of Contents

First define all of the needed parameters and constants, being careful with units.

```
A = 238;                                   % ratio of nuclear mass to neutron mass
a = (0.123*A^(1.0/3.0) + 0.08)*1e-12;      % hard-sphere radius of nucleus, cm
I = 0;                                     % target spin, unitless
J = 0.5;                                   % compound nucleus spin, unitless
E_i = 6.67;                                % location of resonance, eV
Gamma_i  = 0.02752;                        % total resonance width, eV
Gamma_ni = 0.00152;                        % neutron partial width, eV
Gamma_gi = 0.026;                          % radiative capture partial width, eV
c = 2.99792458e10;                         % speed of light in vacuum, cm/s
m = 939.57e6/c^2;                          % mass of neutron, eV/c^2 = eV s^2/cm^2
hbar = 4.135667662e-15/(2.0*pi);           % reduced plank's constant, eV s
k = 8.61734e-5;                            % boltzmann constant, eV/K
gJ = (2*J+1)/(2*(2*I+1));                  % statistical spin factor, unitless
```

0k Single-Level Breit-Wigner Capture and Elastic Scattering Cross Sections

First, create a function to calculate the neutron wavelength as a function of energy:

$$\lambda = \frac{A+1}{A}\frac{\hbar}{\sqrt{2Em}}$$

```
wavelength = @(E) (A+1)/A*hbar./sqrt(2.0*E*m); % eV s/sqrt(eV eV s^2 / cm^2) = cm
```

Now create functions to calculate σ_0 and the s-wave potential cross section, σ_p^0, as functions of energy, where

$$\sigma_0 = 4\pi\lambda^2 g_J \frac{\Gamma_{n,1}}{\Gamma_i}$$

and

$$\sigma_p^0 = 4\pi\lambda^2 \sin^2\frac{a}{\lambda}$$

```
sigma0 = @(E) 4.0*pi*wavelength(E).^2*gJ*Gamma_ni/Gamma_i;  % cm^2
sigmap = @(E) 4.0*pi*wavelength(E).^2.*sin(a./wavelength(E)).^2;
```

Now we have everything in place to calculate the the capture and elastic scattering cross sections. Rather than doing the actual calculation here, I am going to create two functions that will do the calculation as a function of energy. The function `sigma_g` will calculate the capture cross section given by

$$\sigma_g(E) = \sigma_0(E)\frac{\Gamma_{g,i}\Gamma_i}{\Gamma_i^2 + 4(E - E_i)^2}$$

while the function `sigma_e` will calculate the elastic scattering cross section given by

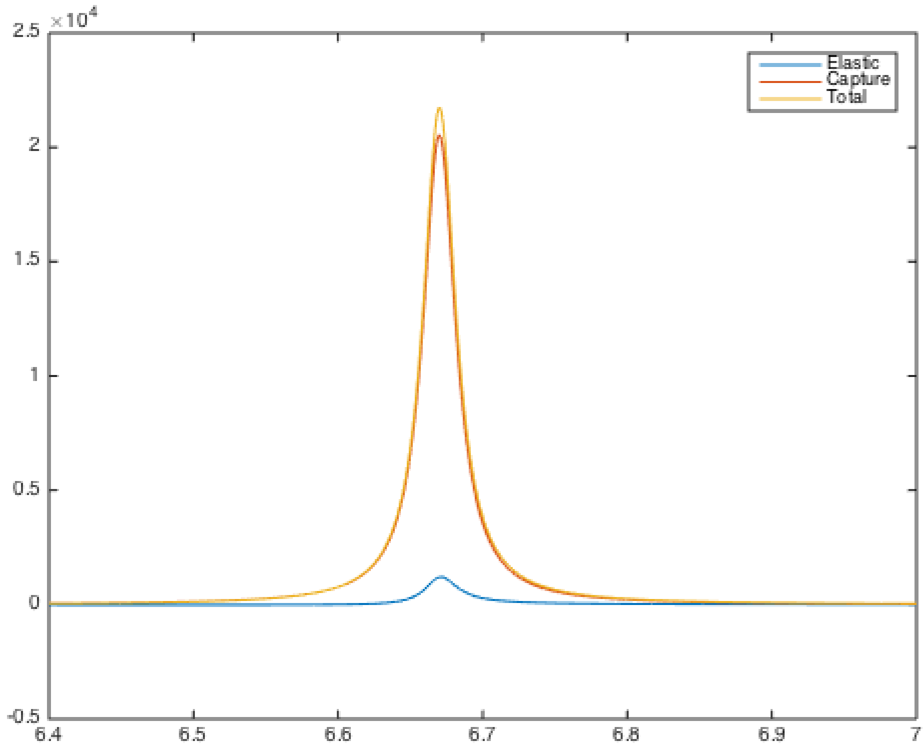
$$\sigma_e(E) = \sigma_p^0(E) + \sigma_0(E)\left[\frac{2}{\Gamma_i}(E - E_i)\sin 2\frac{a}{\lambda} + \frac{\Gamma_{n,i}}{\Gamma_i} - 2\sin^2\frac{a}{\lambda}\right]\frac{\Gamma_i^2}{\Gamma_i^2 + 4(E - E_i)^2}$$

The code implementing these functions is given below

```
function sigma_g = sigma_g(E,Gamma_gi,Gamma_i,E_i,sigma0)

             sigma_g = sigma0(E)*Gamma_gi*Gamma_i./(Gamma_i^2 + 4.0*(E-E_i).^2);

end

function sigma_e = sigma_e(E,a,Gamma_ni,Gamma_i,E_i,sigma0,sigmap,wavelength)
  phi0 = a./wavelength(E);
  sigma_e = sigmap(E).^2 + ...
            sigma0(E).*(2/Gamma_i*(E-E_i).*sin(2.0*phi0) + ...
                        Gamma_ni/Gamma_i - 2.0*sin(phi0).^2)*Gamma_i^2./(Gamma_i^2
end
```

Now calculate and plot:

```
E = linspace(6.4,7.0,1000);
sigmae0 = sigma_e(E,a,Gamma_ni,Gamma_i,E_i,sigma0,sigmap,wavelength)*1.0e24;  % el
sigmag0 = sigma_g(E,Gamma_gi,Gamma_i,E_i,sigma0)*1.0e24;  % capture cross section,
sigmat0 = sigmag0+sigmae0;    % total cross section, barns

elastic = plot(E,sigmae0); hold on;
capture = plot(E,sigmag0);
total   = plot(E,sigmat0); hold off;
legend('Elastic','Capture','Total')
```



Doppler Broadened Cross Sections

Now let's calculate Doppler broadened cross sections. We will do this using the $\psi - \phi$ formulation under the assumption $\alpha = 0$. Thus we need to evaluate

$$\psi(u,\beta) = \frac{1}{\beta\sqrt{\pi}} \int_{-\infty}^{\infty} dv \frac{1}{1+v^2} \exp\left[-\frac{(v-u)^2}{\beta^2}\right]$$

and

$$\phi(u,\beta) = \frac{1}{\beta\sqrt{\pi}} \int_{-\infty}^{\infty} dv \frac{v}{1+v^2} \exp\left[-\frac{(v-u)^2}{\beta^2}\right]$$

where $u = \frac{2}{\Gamma_i}(E - E_i)$, $\beta = \frac{2\Gamma_D}{\Gamma_i}$ and $\Gamma_D = 2\sqrt{\frac{E_i kT}{A}}$.

The ψ and ϕ functions are evaluated using a Gauss-Hermite quadrature. This form of evaluation is only accurate at very low energies due to the shape of the integrand (which can become highly peaked). I am using 200 quadrature points to get rid of the oscillations that result from a poor approximation. To get the integrals in the right form for the quadrature we should make the substitution $x = \frac{v-u}{\beta}$, which leads to

$$\psi(u,\beta) = \frac{1}{\sqrt{\pi}} \int_{-\infty}^{\infty} dx \frac{1}{1+(u+x\beta)^2} e^{-x^2}$$

and

$$\phi(u,\beta) = \frac{1}{\sqrt{\pi}}\int_{-\infty}^{\infty} dx \frac{u + x\beta}{1 + (u + x\beta)^2} e^{-x^2}$$

The code for ψ and ϕ are given below.

```
function f = psi_Doppler(u, beta)
    n = 200;
    [x, w] = GaussHermite(n);
    f = 0;
    for i = 1:n
       f = f + 1.0./(1.0 + (x(i)*beta + u).^2)*w(i);
    end
    f = 1.0/sqrt(pi)*f;
end

function f = phi_Doppler(u, beta)
    n = 200;
    [x, w] = GaussHermite(n);
    f = 0;
    for i = 1:n
        f = f + (x(i)*beta + u)./(1.0 + (x(i)*beta + u).^2)*w(i);
    end
    f = 1.0/sqrt(pi)*f;
end
```

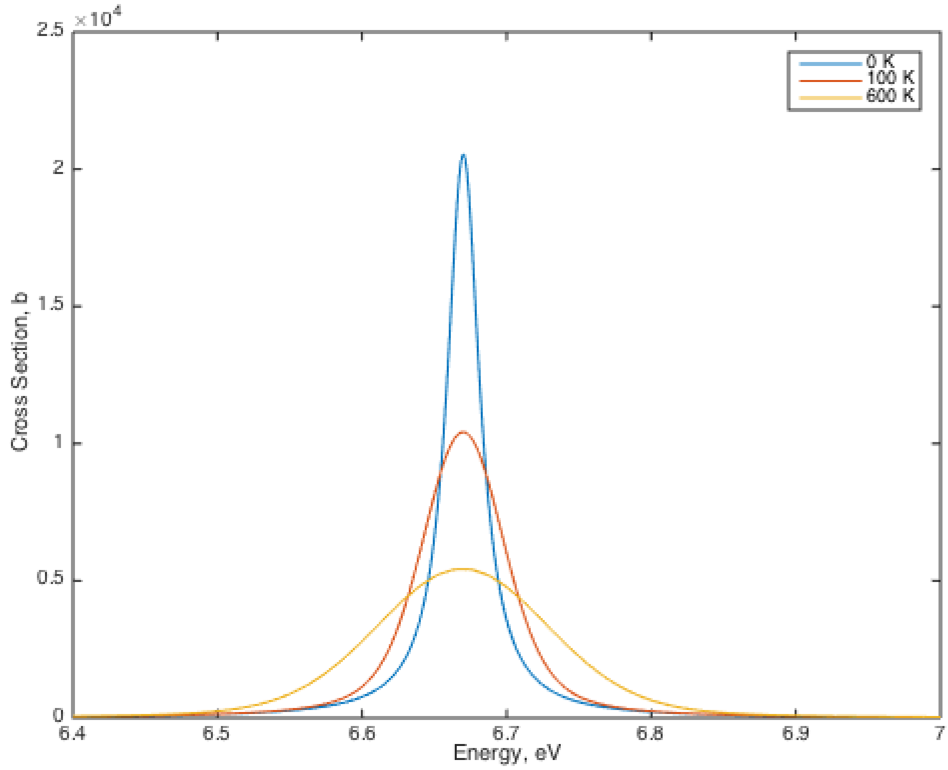
We can now write a function to calculate the Doppler-broadened capture cross section

$$\bar{\sigma}_x(E) = \sigma_0(E)\frac{\Gamma_{x,i}}{\Gamma_i}\psi(u(E),\beta)$$

```
function sigma_g = sigma_g_Doppler(E,Gamma_gi,Gamma_i,E_i,sigma0,T,k,A)
    u = 2.0./Gamma_i*(E-E_i);
    Gamma_D = 2.0*sqrt(E_i*k*T/A);
    beta = 2.0*Gamma_D/Gamma_i;
    sigma_g = sigma0(E).*Gamma_gi/Gamma_i.*psi_Doppler(u,beta);
end
```

Calculate and plot:

```
sigmag100 = sigma_g_Doppler(E,Gamma_gi,Gamma_i,E_i,sigma0,100.0,k,A)*1.0e24;
sigmag600 = sigma_g_Doppler(E,Gamma_gi,Gamma_i,E_i,sigma0,600.0,k,A)*1.0e24;

plot(E,sigmag0);   hold on
plot(E,sigmag100)
plot(E,sigmag600); hold off
legend('0 K','100 K','600 K')
xlabel('Energy, eV')
ylabel('Cross Section, b')
```



The Doppler broadened scatter cross section is

$$\bar{\sigma}_e(E) = 4\pi a^2 + \sigma_0(E)\frac{2a}{\lambda}\phi(u(E),\beta) + \sigma_0(E)\frac{\Gamma_{n,i}}{\Gamma_i}\psi(u(E),\beta)$$

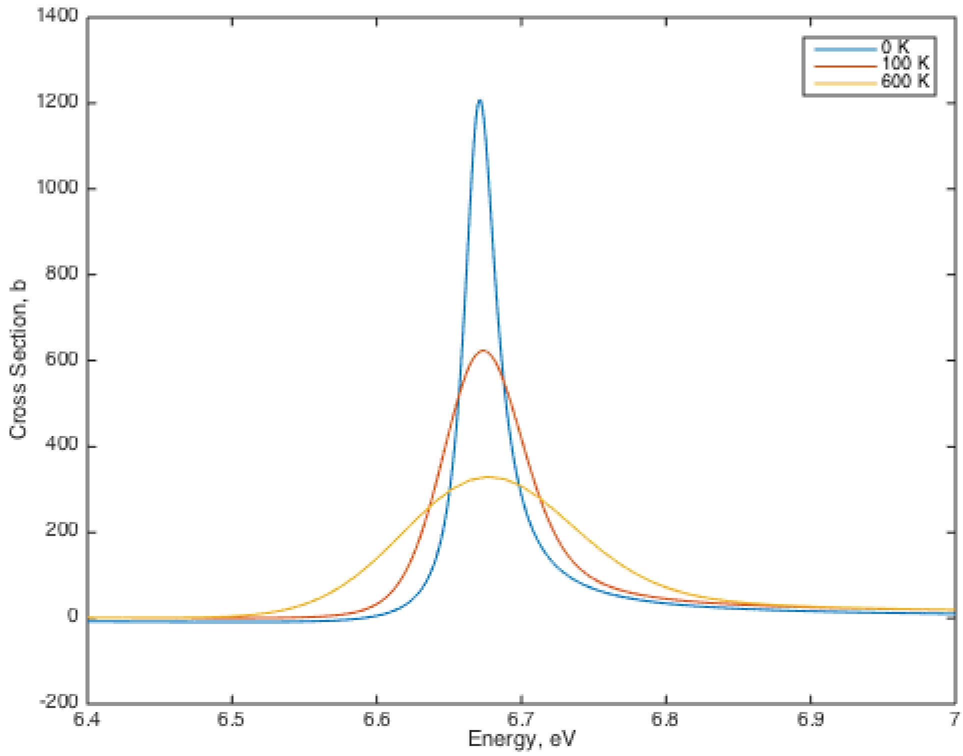
which I implement in the following function.

```
function sigma_e = sigma_e_Doppler(E,a,Gamma_ni,Gamma_i,E_i,sigma0,wavelength,T,k,
    u = 2.0./Gamma_i*(E-E_i);
    Gamma_D = 2.0*sqrt(E_i*k*T/A);
    beta = 2.0*Gamma_D/Gamma_i;
    sigma_e = 4.0*pi*a^2 + ...
              sigma0(E).*(2.0*a./wavelength(E).*phi_Doppler(u,beta) ...
                          + Gamma_ni/Gamma_i*psi_Doppler(u,beta));
end
```

Calculate and plot:

```
sigmae100 = sigma_e_Doppler(E,a,Gamma_ni,Gamma_i,E_i,sigma0,wavelength,100,k,A)*1.
sigmae600 = sigma_e_Doppler(E,a,Gamma_ni,Gamma_i,E_i,sigma0,wavelength,600,k,A)*1.

plot(E,sigmae0);   hold on
plot(E,sigmae100)
plot(E,sigmae600); hold off
legend('0 K','100 K','600 K')
xlabel('Energy, eV')
```

```
ylabel('Cross Section, b')
```



Flux Spectrum in a Resonance

Let's look at this resonances effect on the flux spectrum. For neutrons to be slowing down past the resonance, we need a moderating material. Let's use hydrogen and calculate its potential cross section using the hard-sphere formula for nuclear radius. I will also define the ratio of moderator number density to absorber density as 115.

```
sigmaSM = 4.0*pi*(0.123 + 0.08)^2;   % barns
NMtoNR = 115.0;
```

Now use the narrow resonance approximations to estimate the the spectrum in and around the resonance. Given the current assumptions the narrow resonance approximation can be written

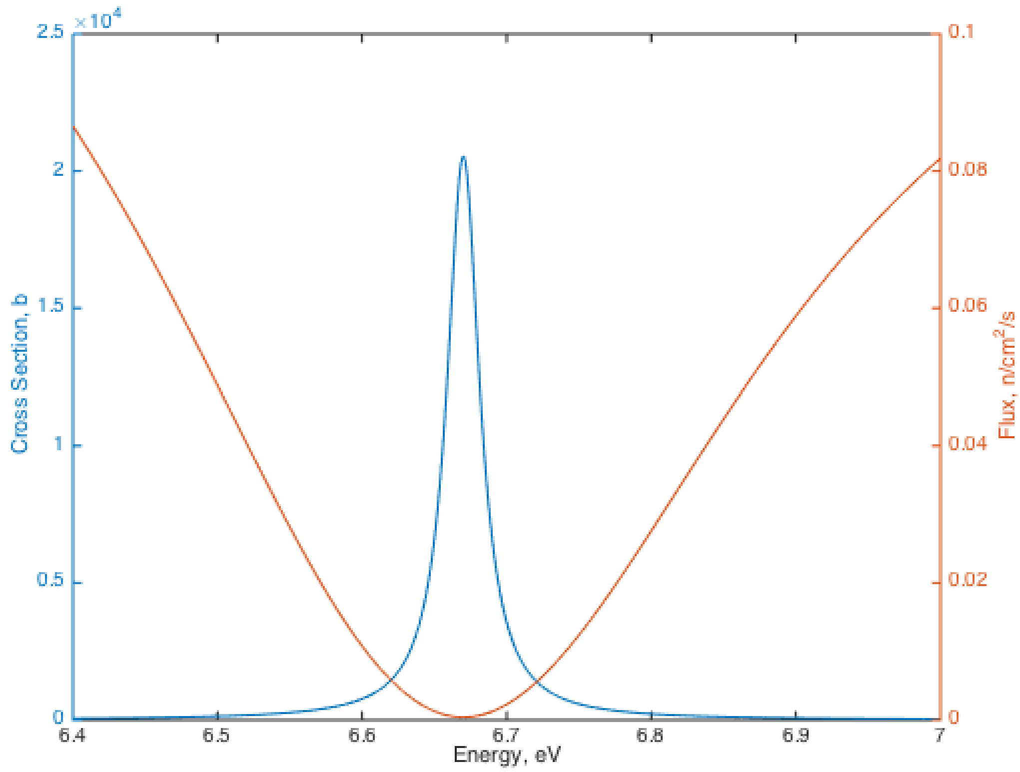
$$\phi_{NR}(E) = \frac{\frac{N^M}{N^{res}}\sigma_s^M + \sigma_p^{0,res}}{\left[\frac{N^M}{N^{res}}\sigma_s^M + \sigma_t^{res}(E)\right] E}$$

where $\phi_{NR}(E)$ is the flux spectrum, not to be confused with the Doppler-ϕ function!

```
sigmaSRes = sigma_e(E,a,Gamma_ni,Gamma_i,E_i,sigma0,sigmap,wavelength)*1.0e24; % b
sigmaARes = sigma_g(E,Gamma_gi,Gamma_i,E_i,sigma0)*1.0e24;   %barns
sigmaTRes = sigmaARes + sigmaSRes;

phi_NR = (NMtoNR*sigmaSM + sigmap(E))./((sigmaTRes + NMtoNR*sigmaSM).*E);
```

Let's plot the flux superimposed over the capture cross section to make sure everything looks right.

```
[hAx,hSigma,hPhi] = plotyy(E,sigmaARes, E,phi_NR);
xlabel('Energy, eV')
ylabel(hAx(1),'Cross Section, b') % left y-axis
ylabel(hAx(2),'Flux, n/cm^2/s') % right y-axis
```



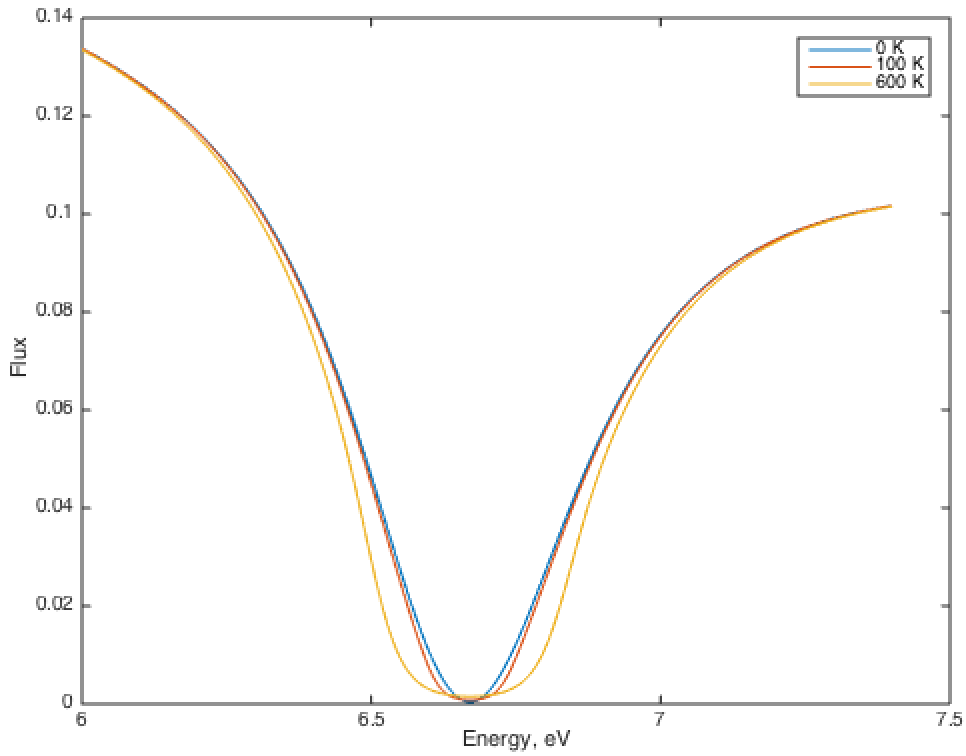
Now let's look at the effect of Doppler broadening. I will use the narrow resonance approximation with the 0 K and Doppler broadened cross sections from the last section.

```
EE = linspace(6.0,7.4,1000);
sigmaTRes0 = (sigma_g_Doppler(EE,Gamma_gi,Gamma_i,E_i,sigma0,0.0,k,A) ...
            + sigma_e_Doppler(EE,a,Gamma_ni,Gamma_i,E_i,sigma0,wavelength,0.0,k,A)
sigmaTRes100 = (sigma_g_Doppler(EE,Gamma_gi,Gamma_i,E_i,sigma0,100.0,k,A) ...
            + sigma_e_Doppler(EE,a,Gamma_ni,Gamma_i,E_i,sigma0,wavelength,100.0,k,
sigmaTRes600 = (sigma_g_Doppler(EE,Gamma_gi,Gamma_i,E_i,sigma0,600.0,k,A) ...
            + sigma_e_Doppler(EE,a,Gamma_ni,Gamma_i,E_i,sigma0,wavelength,600.0,k,

phi_NR0 = (NMtoNR*sigmaSM + sigmap(E))./((sigmaTRes0 + NMtoNR*sigmaSM).*EE);
phi_NR100 = (NMtoNR*sigmaSM + sigmap(E))./((sigmaTRes100 + NMtoNR*sigmaSM).*EE);
phi_NR600 = (NMtoNR*sigmaSM + sigmap(E))./((sigmaTRes600 + NMtoNR*sigmaSM).*EE);
```

And plot...

```
plot(EE,phi_NR0, EE,phi_NR100, EE,phi_NR600)
legend('0 K','100 K','600 K')
xlabel('Energy, eV')
```

```
ylabel('Flux')
```



Neutron Capture Rates

The capture rate for a given resonance capture cross section $\sigma_g(E)$ is

$$R = \int_0^\infty N^{res} \sigma_g(E) \phi(E) dE.$$

Here I will pick $N^{res} = 1.0$ inverse barn-cm, so that if the capture cross section is in barns and the flux is in units of inverse cm^2-sec then R will have units of inverse cm^3.

Because I calculated the flux spectra on a uniform energy grid, then I can approximate the capture integral using

$$R \approx h \sum_j \sigma_g(E_j) \phi(E_j)$$

where h is the energy spacing and j is the index into my energy points. Of course, the total energy range should be sufficiently wide to include all of the significant capture region.

```
h = EE(2) - EE(1);
fprintf(1,'Capture rate at 0 K = %7.4f \n', sum(phi_NR0.*sigma_g_Doppler(EE,Gamma_
fprintf(1,'Capture rate at 0 K = %7.4f \n', sum(phi_NR100.*sigma_g_Doppler(EE,Gamm
fprintf(1,'Capture rate at 0 K = %7.4f \n', sum(phi_NR600.*sigma_g_Doppler(EE,Gamm
```

```
Capture rate at 0 K =  5.1424
Capture rate at 0 K =  5.2068
Capture rate at 0 K =  5.5243
```

Published with MATLAB® R2014b