HW 1
Solution Set

1.) The 1-dimensional Gaussian wave function is $\Psi(x) = \left(\frac{1}{\pi}\right)^{1/4} e^{-x^2/2}$, which

Fourier transforms to $\Psi(k) = \left(\frac{1}{\pi}\right)^{1/4} e^{-k^2/2}$.

a. Determine the particle probability density (in x) and plot it as a function of x.
b. Determine $\Delta x = \sqrt{\langle x^2 \rangle - \langle x \rangle^2}$, where $\langle x^2 \rangle = \int_{-\infty}^{\infty} \Psi^* x^2 \Psi dx$.
c. Calculate $\Delta k = \sqrt{\langle k^2 \rangle - \langle k \rangle^2}$.
d. What is $\Delta x \Delta k$ equal to?

Gaussian Wave Function

The Gaussian wave function (in one dimension) is given by

$$\psi(x) = \left(\frac{1}{\pi}\right)^{\frac{1}{4}} e^{-x^2/2}.$$

The Fourier transform of the Gaussian wave function is

$$\hat{\psi}(k) = \left(\frac{1}{2\pi}\right)^{\frac{1}{2}} \int_{-\infty}^{\infty} \psi(x) e^{-ikx} dx = \left(\frac{1}{2\pi}\right)^{\frac{1}{2}} \left(\frac{1}{\pi}\right)^{\frac{1}{4}} \int_{-\infty}^{\infty} e^{-(x^2/2)-ikx}\, dx,$$

an integral with a general solution of the form

$$\int_{-\infty}^{\infty} e^{-p^2x^2 \pm qx}\, dx = \frac{\sqrt{\pi}}{p}\, e^{q^2/4p^2},$$

which evaluates to

$$\hat{\psi}(k) = \left(\frac{1}{2\pi}\right)^{\frac{1}{2}} \left(\frac{1}{\pi}\right)^{\frac{1}{4}} (2\pi)^{\frac{1}{2}} e^{-k^2/2} = \left(\frac{1}{\pi}\right)^{\frac{1}{4}} e^{-k^2/2},$$

and has the same form as the position-space function.

The square of the Gaussian wave function is the probability density, given by

$$|\psi(x)|^2 = \left(\frac{1}{\pi}\right)^{\frac{1}{2}} e^{-x^2}$$

in (one-dimensional) position space, and by

$$\left|\hat{\psi}(k)\right|^2 = \left(\frac{1}{\pi}\right)^{\frac{1}{2}} e^{-k^2}$$

in (one-dimensional) momentum space.

If we consider the uncertainty in the measurement of the position and momentum of a particle described by the Gaussian wave function, as the particle travels along the x-axis, we find that

$$\Delta x = \sqrt{< x^2 > - < x >^2}\,,$$

$$\langle x \rangle = \int x\left|\psi(x)\right|^2 dx = \left(\frac{1}{\pi}\right)^{\frac{1}{2}} \int_{-\infty}^{\infty} x e^{-x^2} dx = 0\,,$$

given that $\langle x \rangle$ is an odd function evaluated over an even interval, and

$$\left\langle x^2 \right\rangle = \int x^2 \left|\psi(x)\right|^2 dx = \left(\frac{1}{\pi}\right)^{\frac{1}{2}} \int_{-\infty}^{\infty} x^2 e^{-x^2} dx\,,$$

where the integral evaluates to

$$\int_0^{\infty} x^{2n} e^{-px^2} dx = \frac{(2n)!}{2^n n!}\left(\frac{1}{2(2p)^n}\right)\sqrt{\frac{\pi}{p}}\,,$$

$$\left\langle x^2 \right\rangle = 2\left(\frac{1}{\pi}\right)^{\frac{1}{2}} \int_0^{\infty} x^2 e^{-x^2} dx = 2\left(\frac{1}{\pi}\right)^{\frac{1}{2}} \frac{1}{4}(\pi)^{\frac{1}{2}} = \frac{1}{2}\,.$$

Therefore the uncertainty in the particle's position is

$$\triangle x = \sqrt{< x^2 > - < x >^2} = \frac{1}{\sqrt{2}}.$$

For the uncertainty in the particle's momentum, by similar means, we have

$$\triangle k = \sqrt{< k^2 > - < k >^2},$$

$$\langle k \rangle = \int k \left| \hat{\psi}(k) \right|^2 dk = \left(\frac{1}{\pi}\right)^{\frac{1}{2}} \int_{-\infty}^{\infty} k e^{-k^2} dx = 0,$$

$$\langle k^2 \rangle = \int k^2 \left| \hat{\psi}(k) \right|^2 dk = \int_{-\infty}^{\infty} k^2 e^{-k^2} dx = 2\left(\frac{1}{\pi}\right)^{\frac{1}{2}} \left(\frac{1}{4}\right) (\pi)^{\frac{1}{2}} = \frac{1}{2},$$

$$\triangle k = \sqrt{< k^2 > - < k >^2} = \frac{1}{\sqrt{2}}.$$

The product of the uncertainties $\triangle x \triangle k = \frac{1}{2}$ is consistent with the de Broglie form of the uncertainty principle

$$\triangle x \triangle k \geq \frac{1}{2},$$

noting that $\triangle x \triangle k$ has its minimum state when the wave function is of the form

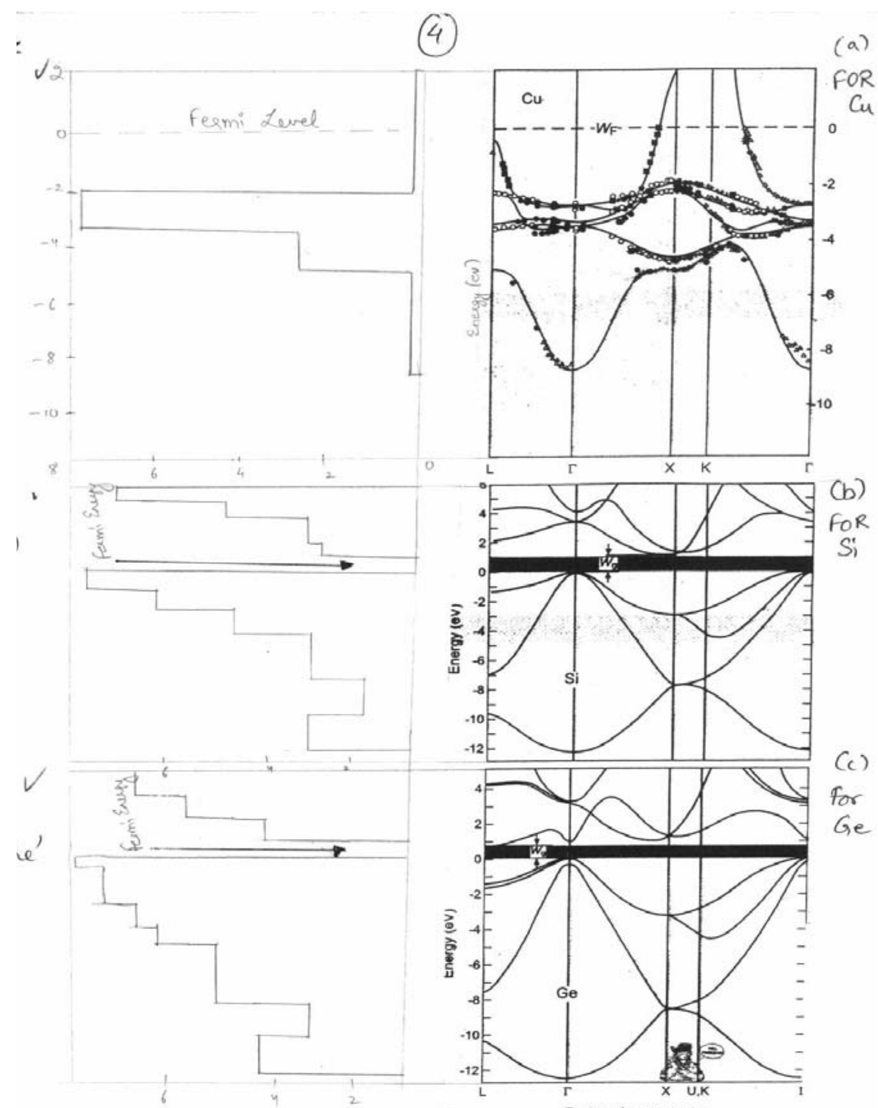
$$\psi(x) = \left(\frac{1}{\pi}\right)^{\frac{1}{4}} e^{-x^2/2},$$

or of the general form (for the one-dimensional case)

$$\psi(x) = \left(\frac{1}{\pi a^2}\right)^{\frac{1}{4}} e^{-x^2/2a^2},$$

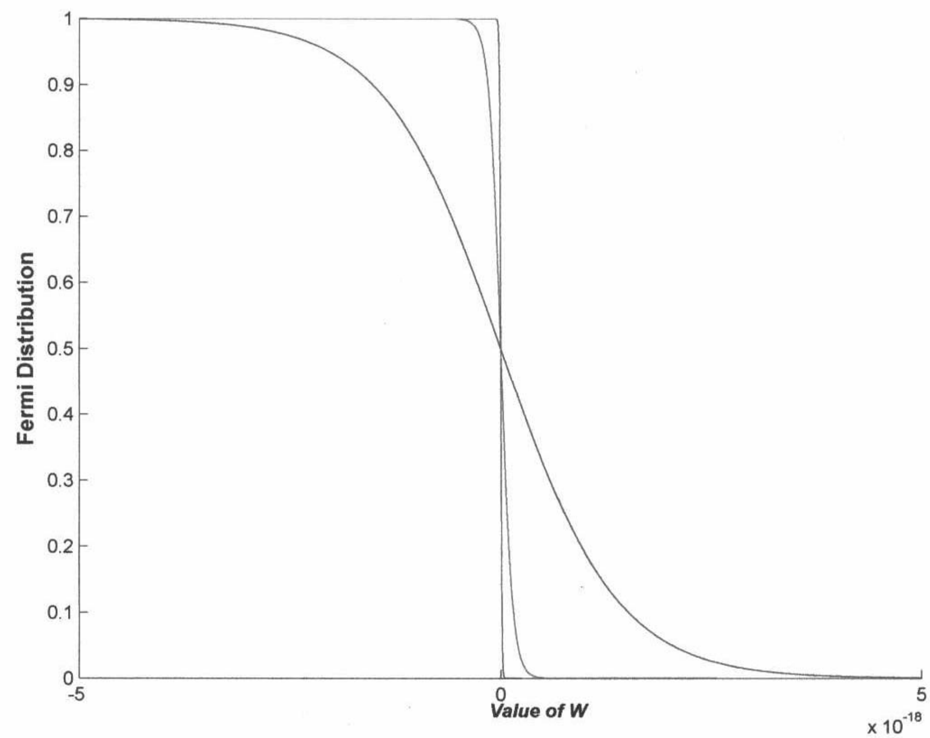
where $a = \pm\sqrt{1}$.

2.) Using figures 5 and 6 in the textbook by Waser, sketch the density of states in the vicinity of the Fermi level for Cu, Ge, and Si. Show explicitly the approximate locations of the Fermi energy and conduction and valence band edges, where appropriate.



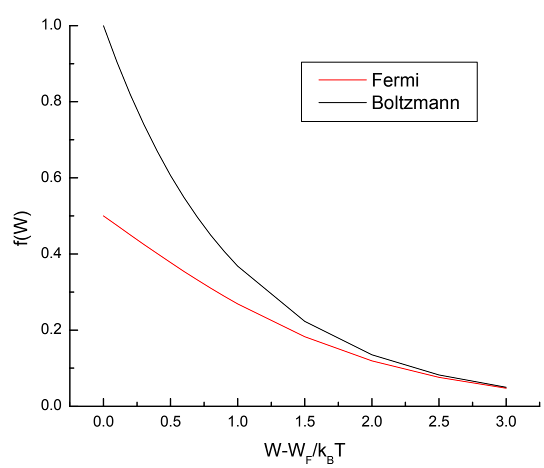
Thanks to Bhumika Chhabra!

3.) Plot the Fermi distribution function as a function of W, for a series of absolute temperatures, 500K, 5 x 10^3 K, 5 x 10^4K, assuming that $W_f/k_B = 0.5$. At approximately what temperature can the Fermi distribution function be approximated by the Boltzmann distribution function?



The squarest distribution is 500K, then 5000K, and then 50,000K.

Fermi statistics can only be approximated at high energies (i.e. large W) at high temperatures. See plot below.



4. Estimate the time between collisions for Na at room temperature, assuming that the electron's effective mass is the actual mass of the electron. What are the electrons colliding with?

The resistivity of Na at room temperature (273 K) is 4.2 x 10^{-6} ohm-cm.
The conductivity of Na is 0.24 x 10^{8} (ohm-m)$^{-1}$. The conductivity is equal to $e^2 \tau n / m_e$.
Assuming 1 electron/atom, and the density of Na is 0.97 g-cm^{-3}, its molecular weight is 23 g/mole, yields 2.5 x 10^{28} electrons/m^3. The time between collisions is then $\sigma m_e / e^2 n$ or [0.24 x 10^{8} (ohm-m)$^{-1}$] [9.1 x 10^{-31} kg]/[1.6 x 10^{-19} C]^2[2.5 x 10^{28} electrons/m^3] or 3 x 10^{-14} seconds (very quick). It turns out that this results in a mean free path of between 1 and 10 Å.

The collisions are between other electrons, ion cores, and vibrations (phonons).