Physics 240B: Homework Problem Set 5
Due: February 14, 2008

1. Numerical Treatment of Debye-Waller Factor. 35 points.
In the earlier problem dealing with the DW factor, which gives the mean-square displacement of an atom and its temperature dependence, the Bose-Einstein thermal occupation function had to be dealt with carefully because of its divergence at $\omega \to 0$ at any non-zero temperature ($\hbar = 1$):

$$n(\beta\omega) = \frac{1}{e^{\beta\omega} - 1} \to \frac{1}{\beta\omega} + ...$$

This divergence can make the integral $\int_0^{\omega_D} .....d\omega$ difficult to handle, and especially difficult to approximate.

The divergence is easy to deal with numerically. Write

$$n(x) = [n(x) - \frac{1}{x}] + \frac{1}{x} \equiv p(x) + \frac{1}{x}.$$

Now the first term approches a finite limit as $x \to 0$ and is well-behaved everywhere else so it can be integrated (at least numerically). And the second term is algebraically simple and, combined with the simple integrands that arise, it can be integrated analytically. So use this separation ("trick") to solve the problem. This problem requires writing a simple integration code (or finding one somewhere.)

(i) Obtain analytically the limiting value of $p(x)$ as $x \to 0$; of course $x = \beta\omega$ in our problem.

(ii) Plot $p(\beta\omega)$ from zero to ω_D for $T/\theta_D = 0.01, 0.05, 0.1, 0.5, 1$. (Of course, do not try to evaluate $p(x = 0)$ from the formula, use a slightly non-zero value of the argument.

(iii) The DW factor involves the integral

$$A \int_0^{\omega_D} d\omega \frac{\omega^j}{\omega} n(\beta\omega)$$

where A gathers all constants, ω^j is the variation of the phonon density of states (different values of the integer j in different dimensions), and ω in the denominator is from the DW integral. The k-sum has been converted into an integral over ω.

Use the separation $n(x) = p(x) + 1/x$ above to determine for which relevant values of j (which dimensions) the integral converges. You should find that it is only for three dimensions; what value of j is this?

Then, insert the separation into the integral, the last part is a simple analytic result. Write a code to do the numerical integration of the first part. Once the code is written it should be quick, so you can calculate the resulting function for any value of T (not too close to zero). Plot the total answer (setting A=1) for T/θ_D=0.01 - 1.0 in steps of 0.01.

(iv) Now (you're doing the problem for 3 dimensions, right?) insert all the constants properly to obtain $u_{rms} = \sqrt{< u^2(T) >}$. Plot the results with units labeled for two very different cases: (a) diamond, $\theta_D = 2000$ K (with mass of carbon), and (b) Pb, θ_D=100 K (with mass of Pb). Use absolute temperature units (K) and absolute distance units (10^{-2} Å should be reasonable) for the plots.