ECE215A/Materials206A Winter 2009
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HW#1 Solutions

(1) **Solid Properties**. Inspecting the Table 2.2 in Kittel, and other sources (see for example, http://www.physicsofmatter.com/Edition2/Download/Tables/pdf/Tab07.pdf):

(a) lowest compressibility,
diamond form of C, $\kappa = 2.26 \times 10^{-12}$ m^2/n ;

(a) highest compressibility
Cs , $\kappa = \sim 500 \times 10^{-12}$ m^2/n (but barely a solid at 300 K, $T_{melt} = 301.6$ K !)

(b) lowest expansivity
W , $\alpha = 4.5 \times 10^{-6}$ K^{-1} ;

(b) highest expansivity
Cd and Zn , $\alpha \approx 30 \times 10^{-6}$ K^{-1}

(from above Website, Table 7.7: α is linear expansivity; volume expansivity, $\beta = 3\alpha$)

(c) lowest thermal conductivity
S, K = 0.15 W/K-m ;

(c) highest thermal conductivity
diamond form of C, K=700-1700 W/K-m

(d) lowest electrical conductivity
S, $\sigma = 5 \times 10^{-16}$ S/m

(d) highest electrical conductivity
Ag, $\sigma = 6.2 \times 10^{7}$ S/m

3. **Quantum Well**. (a) Defining $U_1 = -\Delta U/2$ and $U_2 = \Delta U/2$, we get

$$f(U_1) = \frac{\exp(-U_1/k_BT)}{\exp(-U_1/k_BT)+\exp(-U_2/k_BT)} = \frac{\exp(\Delta U/2k_BT)}{\exp(\Delta U/2k_BT)+\exp(-\Delta U/2k_BT)}$$

And: $$f(U_2) = \frac{\exp(-U_2/k_BT)}{\exp(-U_1/k_BT)+\exp(-U_2/k_BT)} = \frac{\exp(-\Delta U/2k_BT)}{\exp(\Delta U/2k_BT)+\exp(-\Delta U/2k_BT)}$$

Relative probability is $f(U_2)/f(U_1) = \exp(-\Delta U/k_BT)$, which $\to 0$ as $T \to 0$, and $\to 1$ as $T \to \infty$

(b) $$\langle U\rangle = \frac{U_1\exp(-U_1/k_BT)+U_2\exp(-U_2/k_BT)}{\exp(-U_1/k_BT)+\exp(-U_2/k_BT)} = \frac{(-\Delta U/2)\exp(\Delta U/2k_BT)+(\Delta U/2)\exp(-\Delta U/2k_BT)}{\exp(\Delta U/2k_BT)+\exp(-\Delta U/2k_BT)}$$

$= -(\Delta U/2)\tanh(\Delta U/2k_BT)$ $\qquad \langle U\rangle_{tot} = N\langle U\rangle = = -N(\Delta U/2)\tanh(\Delta U/2k_BT)$

(c) $C_V = d\langle U\rangle tot/dT = N(\Delta U)^2/(4k_BT^2)\,\mathrm{sech}^2(\Delta U/2k_BT) = N(\Delta U)^2/(4k_BT^2)\cosh^{-2}(\Delta U/2k_BT)$. Knowing that $\cosh(0) = 1$, we see that $C_V \to 0$ as $T \to \infty$. And for very small T, $C_V \propto (T)^{-2}\exp(-\Delta U/k_BT) \to 0$.

5. **Maxwell-Boltzmann**

(a) By definition $\langle v\rangle = \int_v vP(\mathbf{v})d\mathbf{v} = (m/2\pi k_BT)^{3/2}\int_0^{2\pi}\int_0^{\pi}\int_0^{\infty} v\exp(-mv^2/2k_BT)v^2\sin\theta\, dv d\theta d\phi$

$$= 4\pi(m/2\pi k_BT)^{3/2}\int_0^{\infty} v\exp(-mv^2/2k_BT)v^2 dv$$

From tables of Gaussian integrals (or using your favorite symbolic math tool such as Maple or Mathematica), we find $= \int_0^{\infty} v^3\exp(-mv^2/2k_BT)dv = 2(k_BT/m)^2$

So the final result is $\langle v\rangle = [(8k_BT)/(m\pi)]^{1/2} \approx 1.6\,(k_BT/m)^{1/2}$

(b) The "most likely" velocity is where the pdf has a maximum value with respect to all the independent variables. To see this we convert to scalar form $P(\mathbf{v})d\mathbf{v} = (m/2\pi k_BT)^{3/2}\exp(-mv^2/2k_BT)d\mathbf{v} = (m/2\pi k_BT)^{3/2}\exp(-mv^2/2k_BT)v^2\sin\theta\, dv d\theta d\phi$. The most likely velocity is where

$\partial P/\partial v = 0 = (m/2\pi k_BT)^{3/2}\ \{\exp(-mv^2/2k_BT)2v + v^2\exp(-mv^2/2k_BT)\ (-mv/k_BT)\}$. The solution clearly is $v = (2k_BT/m)^{1/2}$. $\approx 1.4\ (k_BT/m)^{1/2}$

(c) The variance follows from the definition $(\Delta\mathbf{v})^2 \equiv \langle(\mathbf{v} - \langle\mathbf{v}\rangle)^2\rangle = \langle\mathbf{v}^2 - 2v\langle\mathbf{v}\rangle + \langle v\rangle^2\rangle = \langle v^2\rangle - \langle v\rangle^2$. By definition $\langle v^2\rangle = 4\pi(m/2\pi k_BT)^{3/2}\int_0^\infty v^4\exp(-mv^2/2k_BT)dv$. But from Gaussian integral tables (or your favorite symbolic math tool), we find $= \int_0^\infty v^4\exp(-mv^2/2k_BT)dv =$ $(3/8)(\pi)^{1/2}(2k_BT/m)^{5/2}$. So after some fortuitous cancellations, $\langle v^2\rangle = (3k_BT/m)$. And thus $\langle v^2\rangle - \langle v\rangle^2 = (k_BT/m)(3 - 8/\pi)$, and $v_{rms} = [\langle v^2\rangle - \langle v\rangle^2]^{1/2} \approx 0.67\ (k_BT/m)^{1/2}$

(d) $M(\mathbf{v}) = \int_0^\pi\int_0^{2\pi} P(\mathbf{v})d\mathbf{v} = (m/2\pi k_BT)^{3/2}\int_0^{2\pi}\int_0^\pi \exp(-mv^2/2k_BT)v^2\sin\theta\, dv d\theta d\phi = 4\pi(m/2\pi k_BT)^{3/2}$ $\exp(-mv^2/2k_BT)v^2dv$. Thus $dM/dv = 4\pi(m/2\pi k_BT)^{3/2}\exp(-mv^2/2k_BT)v^2$ which is plotted below for a free electron and T = 300 K. Here we clearly see the most likely velocity value as the peak of the curve. And the average value is slightly above the peak, consistent with the fact that the averaging process is skewed by the long Gaussian "tail". We also see that the rms deviation (often called the "standard" deviation) represents the range above and below the average value over which the M(v)dv is large. The fact that it is relatively tight allows one to deal with the entire distribution simply by dealing with the most likely or average values exclusively – an approximation behind the kinetic theory that is so useful in the most basic form of transport theory, known as kinetic theory and addressed later on.

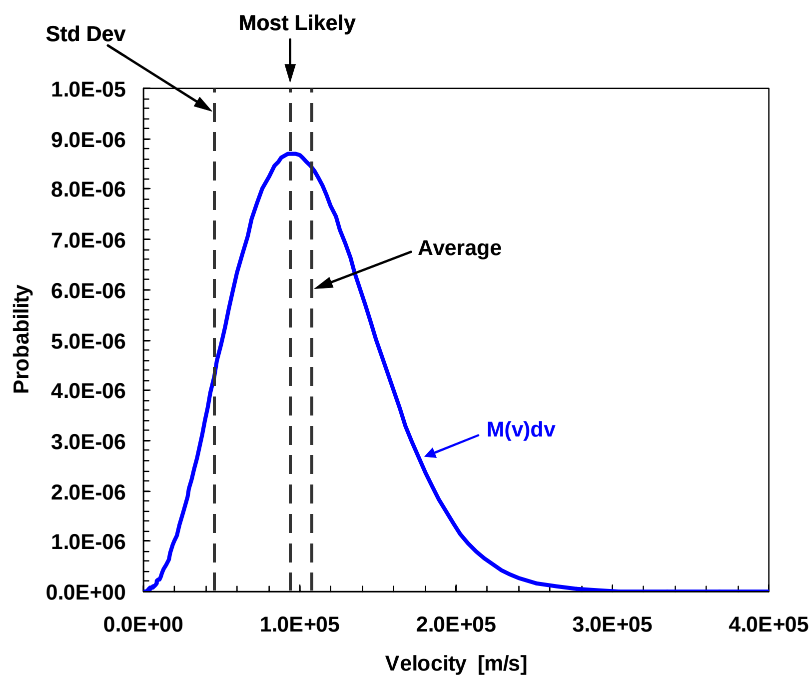

Figure for Problem#5

7. **Bose-Einstein**: To start, the probability of occupancy f_r and mean occupancy Nr of the single-particle quantum state denoted by r are given by

$$f_r = \frac{e^{-(U_r-\mu N_r)/k_BT}}{\sum_s e^{-(U_s-\mu N_s)/k_BT}} \text{ and } < N_r >= \frac{\sum_s N_r e^{-(U_r-\mu N_r)/k_BT}}{\sum_s e^{-(U_s-\mu N_s)/k_BT}}$$

where s indexes all the possible ways particles can occupy the single-particle state r. For Bosons, the denominator (inverse partition function) is an infinite series since the state r can be occupied by an arbitrary number of particles. For example, the first three possible cases are: (1) $N_s = 0$, $U_s = 0$, (2) $N_s = 1$, $U_s = U_r$, (3) $N_s = 2$, $U_s = 2U_r$, (4) $N_s = 3$, $U_s = 3U_r$, so we can write the denominator as an infinite series

$$\sum_s e^{-(U_r-\mu N_r)/k_BT} = \sum_{n=0}^{\infty} e^{-n(U_r-\mu)/k_BT} = \frac{1}{1-e^{-(U_r-\mu)/k_BT}}$$

The numerator is not so obvious until we utilize a trick

$$N_r e^{-(U_r-\mu N_r)/k_BT} = \cdot k_BT \frac{d}{d\mu} e^{-(U_r-\mu N_r)/k_BT}$$

So by exchanging the order of summation and differentiation, we get for the numerator

$$k_BT \frac{d}{d\mu} \sum_s e^{-(U_r-\mu N_r)/k_BT} = k_BT \frac{d}{d\mu} \sum_{n=0}^{\infty} e^{-n(U_r-\mu)/k_BT} = k_BT \frac{d}{d\mu}\left(\frac{1}{1-e^{-(U_r-\mu)/k_BT}} \right)$$

$$= k_BT \frac{d}{d\mu}\left(\frac{1}{1-e^{-(U_r-\mu)/k_BT}} \right) = \frac{e^{-(U_r-\mu)/k_BT}}{(1-e^{-(U_r-\mu)/k_BT})^2}$$

Taking the ratio of the numerator and the denominator, we get

$$< N_r >= \frac{e^{-(U_r-\mu)/k_BT}}{1-e^{-(U_r-\mu)/k_BT}} = \frac{1}{e^{(U_r-\mu)/k_BT} - 1}$$

the famous Bose-Einstein distribution function.