HW#1. Solutions

1. 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

2. (a) Because the copper is isotropic and homogeneous, its linear expansion coefficient α $(1/L)(\partial L/\partial T)$ = 1/3 β. Integrating with respect to L and T, we get $\ln(L_2/L_1) = \beta(T_2-T_1)/3$, or $L_2 = L_1\exp([\beta(T_2-T_1)/3] \approx L_1\{ + [\beta(T_2-T_1)/3]\}$ or $\Delta L \equiv L_2 - L_1 \approx L(1/3)\beta\,\Delta T = 2.05\times10^{-3}$ cm = 20.5 micron

(b) A 20.5 micron compression in the copper block corresponds to $\Delta V = (1- 2.05\times10^{-3})^3 - 1.0 = -6.14\times10^{-3}$ cm^3. The hydrostatic pressure needed for this volume change ΔP is (using same approximation as above): $\Delta P \approx \Delta V/\,(\partial V/\partial P) = \Delta V/(V|\kappa|) = 7.7\times10^{8}$ N/m^2 $\approx 7.7\times10^{3}$ Atm.

3. (a) since the volume is fixed and the temperature is rising, we expect the pressure must rise. To calculate this, we take advantage of the fact that V is an exact differential in T and P. So dV = $\partial V/\partial T|_P\, dT + \partial V/\partial P|_T\, dP = 0$ because of constant volume constraint. So we get dP = $\dfrac{-\partial V/\partial T\,|_P}{\partial V/\partial P\,|_T}$ dT $=(\beta/\kappa)$dT. And if β and κ are assumed constant with respect to temperature (not

a bad approximation, particularly over a 100 K excursion in temperature around 300 K), then by integration $\Delta P = (\beta/\kappa)\ \Delta T$. So for the copper, we get (in MKSA units) $\Delta P = (55\text{x}10^{-6}/0.7\text{x}10^{-11})*100 = 7.9\text{x}10^{8}\ \text{N/m}^2 \approx 7.9\text{x}10^{3}$ Atm. For the Si we get $\Delta P = (8.4\text{x}10^{-6}/1.0\text{x}10^{11})*100 = 8.4\text{x}10^{7}\ \text{N/m}^2 \approx 840$ Atm.

(b) Because of the constant volume, no work is done and the change in energy of the cubes is all by heat, making the heat a total differential. This allows us to obtain the heat input by integrating the specific heat capacity C'_V or $\Delta Q = M\ C_V'\ \Delta T$ where M is the mass of each cube. The densities of Cu and Si are (from Kittel's material Table 1.4) $8.93\text{x}10^3\ \text{kg/m}^3$ and $2.33\text{x}10^3\ \text{kg/m}^3$, respectively. So we find $\Delta Q = 346$ J for Cu and $\Delta Q = 163$ J for Si.

(c) To keep the hydrostatic pressure constant with the rising temperature we consider the exact differential $dP = \partial P/\partial T|_V\ dT + \partial P/\partial V|_T\ dV = 0 = (\beta/\kappa)\ dT + (-1/\kappa)dV$, so that $\Delta V = \beta\ \Delta T = V_0\ \beta\ \Delta T = 5.5*10^{-3}\ \text{cm}^3$ for the Cu, and $8.4*10^{-4}\ \text{cm}^3$ for the Si.

4 (a) From electrostatics we know the potential energy of a neutral (i.e., equal + and – charge) dipole in an electric field is $U = -\mathbf{p}\cdot\mathbf{E}$ where **p** is the dipole moment that, by convention, points between the – and + charges and has magnitude $q\cdot d$ where q is the dipole charge and d is the charge separation $= a/(2)^{1/2}$ according to the Figure below. So for the E oriented as shown between the – and + charges, the potential energy of the four possible interstitial sites as enumerated is:

$U_1 = -\mathbf{p}_1\cdot\mathbf{E} = \mathbf{0}$ (since $\mathbf{p}_1$ and **E** are perpendicular); $U_2 = -\mathbf{p}_2\cdot\mathbf{E} = -eaE/(2)^{1/2}$

$U_3 = -\mathbf{p}_3\cdot\mathbf{E} = eaE/(2)^{1/2}$; $U_4 = -\mathbf{p}_4\cdot\mathbf{E} = 0$ (since $\mathbf{p}_4$ and **E** are perpendicular)

By assuming M-B Statistics, we can thus write probability of occupancy of the *ith* dipole level $P_i = Ce^{-U_i/k_BT}$ where $C = \left(\sum_{i=1}^{4} e^{-U_1/k_BT}\right)^{-1}$ is the normalization constant.

Exponential factors: Dipole (1): $e^{-U_1/k_BT} = e^{-0} = 1$; Dipole (2): $e^{-U_2/k_BT} = e^{\left(\frac{eaE}{\sqrt{2}}\right)/k_BT}$

Dipole (3): $e^{-U_2/k_BT} = e^{-\left(\frac{eaE}{\sqrt{2}}\right)/k_BT}$; Dipole (4) : $e^{-U_3/k_BT} = e^{-0} = 1$

$C = \{2 + \exp[eaE/(2^{1/2}k_BT)] + \exp[-eaE/(2^{1/2}k_BT)]\}^{-1}$

(b) Substitution of a = 3×10^{-10} m, E = 1×10^{8} V/m, and T = 300 K yields $eaE/(2^{1/2}k_BT) = 0.821$

so C = $(2 + 2.27 + 0.44)^{-1}$ = 0.2123, and we get for the probabilities:

P_1 = 0.212 P_2 = 0.482 P_3 = 0.094 P_4 = 0.212

{Note: $P_1 + P_2 + P_3 + P_4 = 1.0$ as expected for any probability calculation}

5. Maxwell-Boltzmann distribution of velocities

(a) By definition <v> = $\int_{\vec{v}} vP(\mathbf{v})d\mathbf{v} = \int_{\mathbf{v}} vP(\mathbf{v})d\mathbf{v} = (m/2\pi k_BT)^{3/2}\int_0^{2\pi}\int_0^{\pi}\int_0^{\infty} v\exp(-mv^2/2k_BT)v^2\sin\theta dv d\theta d\phi$

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

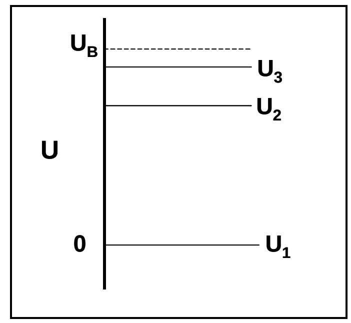
From tables of Gaussian integrals (or using your favorite symbolic math tool such as Maple or Mathematica), we find $=\int_0^{\infty} v^3\exp(-mv^2/2k_BT)dv = 2(k_BT/m)^2$

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

(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 $P(\mathbf{v})d\mathbf{v} = (m/2\pi k_BT)^{3/2}\exp(-mv^2/2k_BT)d\mathbf{v} = (m/2\pi k_BT)^{3/2}\exp(-mv^2/2k_BT)v^2\sin\theta dv d\theta df$. 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(v)dv= $\int_0^{\pi}\int_0^{2\pi} P(v)dv d\theta d\phi = (m/2\pi k_BT)^{3/2}\int_0^{2\pi}\int_0^{\pi}\exp(-mv^2/2k_BT)v^2\sin\theta dv d\theta d\phi = 4\pi(m/2\pi k_BT)^{3/2}\exp(-mv^2/2k_BT)v^2dv$. Thus $dM/dv = 4\pi(m/2\pi k_BT)^{3/2}\exp(-mv^2/2k_BT)v^2$ which is evaluated on the attached Excel spreadsheet and plotted below. 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.



6 (a) Referring to the diagram at right, the Boltzman pdf will always favor the level of lowest total energy, level U_1 in this case. $P_1 = C\exp(-U_1/k_BT) = C\exp(-0U_B/k_BT) = C$, and $C^{-1} = \exp(-U_1/k_BT)+ \exp(-U_2/k_BT)+ \exp(-U_3/k_BT) = \exp(-0/k_BT)+ \exp(-3U_B/4k_BT)+ \exp(-8U_3/9k_BT)$. For $U_B = k_BT$, we get $C^{-1} = 1 + \exp(-3/4) + \exp(-8/9) = 1 + 0.472 + 0.411 = 1.883$ and $P_1 = 1/1.883 = 0.53$

(b) Lowest probability is for U_3, $P_3 = C\exp(-U_3/k_BT) = C\exp(-8U_B/9k_BT)$ with $C^{-1} = \exp(-0/k_BT)+ \exp(-3U_B/4k_BT)+ \exp(-8U_3/9k_BT)$. So for $U_B = k_BT$, $C^{-1} = 1.883$ as before, and $P_3 = 0.411/1.883 = 0.22$.

7. Heat capacity in two level system, energy splitting = $\Delta \cdot k_B$

(a) By Maxwell Boltzmann Statistics

$$< U >= \frac{U_1 e^{-U_1/kT} + U_2 e^{-U_2/k_BT}}{e^{-U_1/k_BT} + e^{-U_2/k_BT}}$$

Set U_1 (arbitrarily) to zero so that $U_2 = k_B\Delta$.

$$< U >= \frac{k_B \Delta e^{-k_B\Delta/k_BT}}{1 + e^{-k_B\Delta/k_BT}} = \frac{k_N \Delta e^{-\Delta/T}}{1 + e^{-\Delta/T}}$$

$$C_\upsilon = \frac{d < U >}{dT} = \frac{\left(1+e^{-\Delta/T}\right)\left(\frac{+\Delta k_B \Delta}{T^2}\right)e^{-\Delta/T} - \left(k_B \Delta e^{-\Delta/T}\right)\left(\frac{+\Delta}{T^2}\right)e^{-\Delta/T}}{\left(1+e^{-\Delta/T}\right)^2}$$

$$C_\upsilon = \frac{+k_B \Delta^2 e^{-\Delta/T} / T^2}{\left(1+e^{-\Delta/T}\right)^2} = \frac{k_B \left(\Delta/T\right)^2 e^{-\Delta/T}}{\left(1+e^{-\Delta/T}\right)^2} = \frac{k_B \left(\Delta/T\right)^2 e^{\Delta/T}}{\left(e^{\Delta/T}+1\right)^2}$$

(b) The plot of the heat capacity in (a) is shown below. By graphical means, we determine that the maximum in C_V occurs at a value of $\Delta/T = 2.06$.

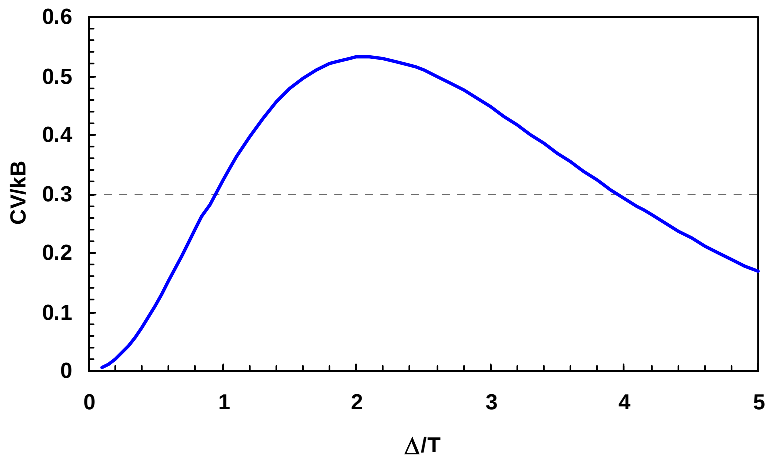


Figure for Problem 7