Practice Problems for Midterm 2, 2017

Problem 1) Fermi Gas and MB gas comparison

A) Gold is a dense metal with density $1.93\times10^4 kg \bullet m^{-3}$ at T = 300K. Calculate its number density (n=N/V) in m^{-3}. Assume that **a gold atom** contributes **one conducting electron**, calculate its Fermi Energy, E_F, in unit of *eV*. Repeat the calculation but with the assumption that **one gold atom** contributes **two conducting electrons**. Compare your answers with the experimental values of 5.53 *eV*, and comment. Molar mass of gold is 197 g•mol^{-1}

B) Use the answer of part A, to calculate the **mean Thermal energy**, $\bar{E} = U/N$, where U is the internal (mean) energy of the system, as given by the equation in the appendix.

C) Assuming that the conducting electrons can be treated a classical ideal (MB) gas, find the **mean thermal energy** at 300K. Explain the discrepancy between the values of $\bar{E}$ obtained in part B and C.

Problem 2) 2D Maxwell-Boltzman Distribution

a) In 2D the speed distribution becomes $f_{2D}\left(v\right)=\beta mv\exp\left(-\beta\frac{mv^2}{2}\right)$ with $v^2=v_x^2+v_y^2$, material. **Briefly explain** the mathematical meaning of $f_{2D}dv$, and explain why the **normalization** of f_{2D} requires $\int_0^\infty f_{2D}\,dv=1$. **Verify** by direct integration that $\int_0^\infty f_{2D}\,dv=1$.

b) Find the average speed in 2D, $\overline{v}$ of a neutron at T = 300K. Data: Mass of neutron in equation sheet. HINT: $\int_0^\infty x^2\exp\left(-ax^2\right)dx=\left(\pi\right)^{1/2}/\left(4a^{3/2}\right)$.

c) Using $\frac{df_{2D}}{dv}=0$ find the most probable speed of a neutron at T = 300K, and compare with your answer in part b.

Problem 3) Vibrational Energy Level of HCl and HBr molecule.

A) Assume that the HCl molecule behaves like a harmonic oscillator with a force constant of 481 N/m. Find the energy (in eV) of its **ground** (n = 0) and **first excited** (n = 1) vibrational states. DATA: For ^{1}H $m_H = 1\text{u}$; ^{35}Cl $m_{Cl} = 35\text{u}$, and $1\ \text{u} = 1.66\times10^{-27}\,kg$. Note the difference between angular frequency ω (in s^{-1}) and $\nu = \omega/2\pi$ (unit Hz).

B) Bromide (^{80}Br $m_{Br} = 80\text{u}$) and Cholrine (^{35}Cl $m_{Cl} = 35\text{u}$) are **group 17** in the periodic table. In one or two sentences, use the previous sentence to justify why HBR molecule should have similar **force constant**, *k*, as HCl. Then sssume *k* are the same, and calculate the **ground state vibrational energy** of HBr.

C) Spectroscopic data found that the transition vibrational frequency of HCl and HBr are $\nu_{HCl} = 8.66\times10^{13}\,Hz$ and $\nu_{HBr} = 7.68\times10^{13}\,Hz$. Is this data consistent with the finding of part B? If the **answer** is **no**, discuss why in **no more than four sentences**.

Problem 4) Rotational spectroscopy The rotational energy of a diatomic molecule is $E_{rot} = \frac{\ell(\ell+1)\hbar^2}{2I}$.

(A) In a photon absorption experiment a diatomic molecule absorbs a photon, and makes a transition from the ℓ rotational state to the $\ell+1$ rotational state. **Show explicitly** that the energy of the photon is $\Delta E_{photon} = \frac{(\ell+1)\hbar^2}{I}$.

(B) A photon of frequency $\nu = 5.1\times10^{11}\,Hz$ is absorbed by the diatomic molecule HBr resulting in a transition from the $\ell = 0$ to the $\ell = 1$ rotational state. Use this information to determine the average bond length of the molecule. For ^{1}H, $m_H = 1$ amu; ^{80}Br, $m_{Br} = 80$amu; where 1 amu $= 1.66\times10^{-27}\,kg$.

(C) Microwave communication systems (such as wireless connection signals) operate over long distances in the atmosphere. Molecular rotational spectra are in the microwave region. Briefly explain why atmospheric gases do not absorb microwaves to any great extent.

Problem 5

Superconductivity In the superfluid state, liquid helium-4 atoms form Bose-Einstein (BE) condensate that forms circulating vortices that do not dissipate (i.e. do not slow down). In the superconducting state, electrons in metals form BE condensate that conduct with no dissipation (the resistance of a superconductor is zero).

(A) Note that electrons are fermions, but liquid helium-4 atoms are bosons. Explain how electrons in superconducting metals form BE condensate. Your explanation (**no more than 4 sentences**) should include the energy gap E_g.

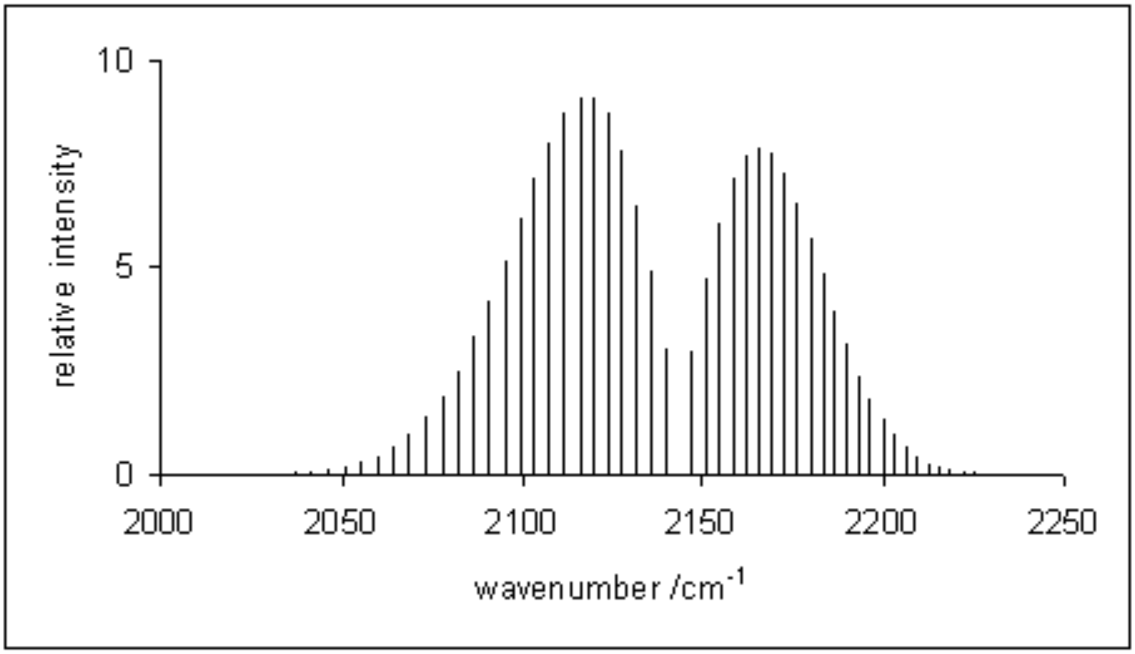
(B) The critical temperature of the superconducting state of Vanadium is $T_C = 5.4K$ and its zero temperature energy gap is $E_g(0) = 15.8 \times 10^{-4}\, eV$. What fraction of electrons in Vanadium is in the superconducting state at temperature $T = 3.0K$? What is the energy gap at $T = 3.0K$? **Note:** assume superconductors obey the same condensate fraction equation as superfluid helium – see equations sheet !!

(C) The **isotope effect** equation states that $M^{0.5}T_C \equiv \text{constant}$, where *M* is the atomic mass of the element. In no more than **four sentences** explain the **underlying physical basis** of this equation.

(D) Vanadium has atomic mass $m_V = 50u$, and Mercury (Hg) has atomic mass $m_{Hg} = 201u$. Use this to estimate the critical temperature of mercury. The actual experimental on Hg is $T_C = 4.2K$. In **no more than three sentences**, discuss whether your calculations validate the **isotope effect** of **superconductivity**.

Problem 6

Ro-vibrational spectrum of CO is shown below:



Use the data above to calculate the bond length and bond spring constant k of CO.
Experimental data: R = 1.13×10^{-10} m, k = 1860 N/m.

Useful Equations **Energy of a photon:** $E = h\nu$ and $\lambda = c/\nu$, where $c = 2.998 \times 10^8 m/s$. **Maxwell-Boltzman 3D speed distribution**.

$F_{MB}(v)dv = 4\pi N\left(m/(2\pi k_B T)\right)^{3/2} v^2 \exp\left(-mv^2/(2k_B T)\right)dv$; root-mean-square speed $v_{rms} = \sqrt{\overline{v^2}} = \sqrt{\frac{3k_B T}{m}}$; mean speed $\bar{v} = \sqrt{\frac{8k_B T}{\pi m}}$

2D speed distribution $f_{2D}(v) = \beta m v \exp\left(-\beta \frac{mv^2}{2}\right)$ with $v^2 = v_x^2 + v_y^2, \bar{v} = \int_0^\infty dv v f_{2D}(v)$

; 3D speed distribution **Ideal gas** $U = \frac{f}{2} k_B T$ f is quadratic degree of freedom; $PV = NK_B T = 2U/3; U = 3Nk_B T/2$.

Rotational Levels: $E_\ell = \frac{L^2}{2I} = \frac{\ell(\ell+1)}{2I}\hbar^2, \ell = 0,1,2\ldots,$ where $I = \mu R^2$ and $\mu = \frac{m_1 m_2}{m_1 + m_2}$. Emission/absorption of photons: i) selection rule $\Delta\ell = \pm 1$; ii) $h\nu = \Delta E_{\ell \leftrightarrow \ell-1}$. $\Delta E_{\ell \leftrightarrow \ell-1} = E_\ell - E_{\ell-1} = \frac{\ell\hbar^2}{I}$.Separation between adjacent lines $\frac{\hbar^2}{I}$. **Vibrational Level** $E_{vibr} = (n + 1/2)\hbar\omega$, $\mathrm{n} = 0,1,2\ldots$,where $\omega = \sqrt{\frac{k}{\mu}}$, and $\mu = \frac{m_1 m_2}{m_1 + m_2}$. $\Delta E_{n+1 \leftrightarrow n} = E_{n+1} - E_n = \hbar\omega$. Absorption and Emission of photons: i) selection rule $\Delta n = \pm 1$; ii) $h\nu = \Delta E_{n+1 \leftrightarrow n}$. **Dissociation Energy (U_0):** $E_{\text{vibr}} = (n + 1/2)\hbar\omega - U_0$.

Ro-vibrational energy is $E_{n,\ell} = \hbar\omega\left(n + \frac{1}{2}\right) + \frac{\hbar^2}{2I}\ell(\ell+1)$, with the first term associated with vibration with quantum number, n = 0, 1, 2, …, and the second with the rotational modes wit quantum numbers $\ell = 0,1,2..$ Selection Rules $\Delta n = n_f - n_0 = \pm 1$ and $\Delta\ell = \ell_f - \ell_0 = 0, \pm 1$, Q-branch $\Delta\ell = 0$; R-branch $\Delta\ell = +1$; P-branch $\Delta\ell = -1$.

Wavenumber $\bar{\nu} = 1/\lambda \rightarrow \bar{\nu} = E_{ph}/hc$, E_{ph} is **photon energy**

Fermi-Dirac(FD) $f_{FD} = 1/\left(e^{(\varepsilon-\mu)/k_B T} + 1\right)$. **Bose-Einstein(BE)** $f_{BE} = 1/\left(e^{(\varepsilon-\mu)/k_B T} - 1\right)$.

Fermi Energy $\varepsilon_F = \left(h^2/2m\right)\left(3N/(8\pi V)\right)^{2/3}$; $T_F = \varepsilon_F / k_B$; $u_F = \sqrt{2\varepsilon_F / m}$; $U = 3N\varepsilon_F / 5$; $PV = 2U/3$

Useful constants: Atomic mass unit (u) 1 u $= 1.66 \times 10^{-27} kg$; electron rest mass $m_e = 9.11 \times 10^{-31} kg$; proton mass $m_p = 1.66 \times 10^{-27} kg$; $e = 1.6 \times 10^{-19} C$; 1 eV $= 1.6 \times 10^{-19} J$; $h = 6.62 \times 10^{-34} J \bullet s = 4.136 \times 10^{-15} eV \bullet s$; $\hbar = 1.055 \times 10^{-34} J \bullet s = 6.582 \times 10^{-16} eV \bullet s$; $k_B = 1.381 \times 10^{-23} J/K = 8.617 \times 10^{-5} eV/K$. $\varepsilon_0 = 8.854 \times 10^{-12} C^2/N \bullet m^2$

Superconductor $M^{0.5}T_c = $ constant, $E_g(0) = 3.54 k_B T_C$,

$E_g(T) = 1.74 E_g(0)\left(1 - (T/T_c)\right)^{1/2}$; $B_C(T) = B_C(0)\left(1 - (T/T_c)^2\right)$.