Time yourself carefully – do not spend most of your time on a single question. Also, give as much written explanation as possible of your reasoning.

1. **Bonding**. (50 points)

Life in Flatlandia – two-dimensional potentials

An electron in a two-dimensional world is confined by an external potential V(x,y) that is 0 for $0 \le x \le a$ and $0 \le y \le a$, and is infinite everywhere else (this does happen in real life – e.g. for an electron trapped in surface nanostructures).

a. (7 points) Write explicitly the stationary Schrödinger equation that is experienced by the electron *in the region inside the confining potential.*

b. (7 points) Find the general solution of this Schrödinger equation by applying the method of separation of variables (explain what you are doing).

c. (7 points) Show that the boundary conditions force a quantization in the energy levels of the electron, and write explicitly the general form of the wavefunctions and energy levels.

d. (7 points) Determine which are the lowest 3 energies that the electron can have, and how many different wavefunctions correspond to each of these energies.

e. (7 points) Determine the wavelength of a photon that is able to excite an electron from the ground state to the first excited state.

f. (10 points) Suppose that we had a different confining potential V(x,y), that along x is 0 for $0 \le x \le a$ and infinite for $x < 0$ and $x > a$, and along y is of the form $\frac{1}{2} ky^2$. What could you say about the solutions of the Schrödinger equation in this case (wavefunctions and energies) ?

g. (5 points) Suppose that we had a different confining potential $V(x,y) = \frac{1}{2} k (x^3+y^3)$. Is this potential Hermitian ? Why ?

Thermodynamics. (50 points)

a. Write an expression for the molar free energy of reaction $\Delta\overline{G}_{rxn}$ for the following systems, in terms of the standard state free energy change $\Delta\overline{G}_{rxn,o}$, the temperature, and other parameters as appropriate. Simplify your expression using the standard approximation for the activity of solid phases if possible.

   i. (7 points) $H_2O_{(g)} + \frac{7}{2}H_2S_{(g)} + 3NO_{2(g)} = 2NH_{3(g)} + \frac{7}{2}SO_{2(g)}$

   ii. (7 points) $Pb_{(s)} + 2Ag^{+}_{(aq)} = Pb^{++}_{(aq)} + 2Ag_{(s)}$

b.

   i. (7 points) Supposing the reaction in part (a) number (ii) occurs in an electrochemical cell, write an expression for the EMF of the battery.

   ii. (7 points) How will the expression change if the lead and silver solutions are ideal?

c. (7 points) Consider a closed system at 560 K and 1 atm pressure, which is at equilibrium with 7 phases in coexistence. If the system has 5 components, could the pressure of the system be changed (*while the temperature remains constant at 560 K*) and maintain all 7 phases in coexistence? (Show why).

d. (15 points) Given the thermodynamic information below, construct a diagram of the Gibbs free energy vs. temperature of a hypothetical material that has 4 different phases: α (a solid phase), β (a solid phase), liquid, and gas. The plot should be qualitatively correct, in terms of the relative shapes, positions, and slopes of the free energy curves. Mark the curves to denote which phase they correspond to, and mark the temperatures of transition.

Given:

- $\Delta\bar{S}^{\alpha\rightarrow\beta} \cong 0$
  $\Delta\bar{S}^{\beta\rightarrow L} = 2.05\frac{\text{J}}{\text{mole}\bullet\text{K}}$
  $\Delta\bar{S}^{L\rightarrow G} = 15.4\frac{\text{J}}{\text{mole}\bullet\text{K}}$

  (i.e., relative to one another, the entropies of the α and β phases are almost the same, the entropy of the liquid phase is moderately larger than the β phase, and the gas phase has a much larger entropy than the liquid phase)

- The temperature of each phase transition is:

  $T^{\alpha\rightarrow\beta} = 250K$
  $T^{\beta\rightarrow L} = 1500K$
  $T^{L\rightarrow G} = 1700K$