1.1	***1.2***	***1.3***	***1.4***	***Total***
5	3	2	12	22

Problem 1: "QQU-QU QQU-QU(antum)" - BLACKPINK

Bulk Sodium is highly conductive due to the small gap between the valence and conduction bands caused by delocalization. This conductivity can be modeled by the particle in a box model. It can be shown that the various energy levels for a particle such as an electron in a 1-dimensional box are given by:

$$E_n = \frac{n^2 h^2}{8mL^2},\ \text{n} = 1, 2, 3\ldots$$

where m is the mass of the particle, L is the length of the box, and n is the energy level. Note that each energy level can be occupied by 2 electrons with opposite spins.

Consider a long chain of exactly 1 x 10^5 Sodium atoms in a straight line. Sodium has an atomic radius of 227 pm. Assume that the electrons are free to move between, but not beyond, the nuclei of the left and rightmost Sodium atoms. The mass of an electron is $m_e = 9.1 \times 10^{-31}$ kg.

1.1 Determine the energy of the highest occupied energy level in joules.
1.2 Write an expression for the HOMO-LUMO energy gap of the system in terms of the quantum number for the highest occupied energy level and then numerically compute it.

The approximate thermal energy of a molecule in a system is given by $E = k_b T$, where $k_b = R/N_a$ is the Boltzmann constant.

1.3 Is there sufficient thermal energy at 100K to excite an electron into a higher energy orbital? Explain with calculations.

The energies of a particle in a 2d box is somewhat more complicated. Now the overall energy state is defined by 2 quantum numbers nx and ny. The energy levels are given by:

$$E_n = \frac{h^2}{8m}\left(\frac{n_x^2}{L_x^2} + \frac{n_y^2}{L_y^2}\right),\ n_x, n_y = 1, 2, 3\ldots$$

Consider now a square sheet of Sodium atoms, with 1 x 10^5 Sodium atoms per side. Again, the same boundary conditions hold: electrons are free to move between, but not beyond, the nuclei of the left and rightmost Sodium atoms.

1.4 Approximate the energy of the highest occupied energy level in this system