Final Project
Submitted by: Mohammad Adnaan

Ques 1. and 2. Effective masses along different directions

Direction	Heavy hole	Light hole
[100]	0.333 m_o	0.0967 m_o
[111]	0.2487 m_o	0.0316 m_o

The values are obtained by curve fitting the energy band diagram within the range $|k_x| < 0.025 \frac{2\pi}{a}$. The curve fitting is done using Matlab curve fitting toolbox. The E-k diagram was fitted into the quadratic equation $E(k) = p_1k^2 + p_2k + p_3$ where p_1, p_2, p_3 are constants.

Now, $\frac{\partial^2 E}{\partial k^2} = 2p_1$

Since unit of E is eV and unit of K is meter^{-1}. So the unit of constant p_1 will be m^2 eV.

Now, $m^* = \hbar^2 \left[\frac{\partial^2 E}{\partial k^2}\right]^{-1}$

or, $\frac{m^*}{m_o} = \frac{\hbar^2}{2p_1 m_o}$

or, $\frac{m^*}{m_o} = \frac{(1.05457\times10^{-34})^2}{2\times1.602\times10^{-19}\times9.10938\times10^{-31}\times p_1}$

or, $\frac{m^*}{m_o} = \frac{3.809981744\times10^{-20}}{p_1}$ …….(i)

Putting the value of p_1 in the above equation, the effective mass of carriers with respect to mass of an electron was directly obtained. For heavy hole effective mass along [100] directions

$p_1 = 1.143\times10^{-19}$ so $\frac{m^*}{m_o} = 0.333$

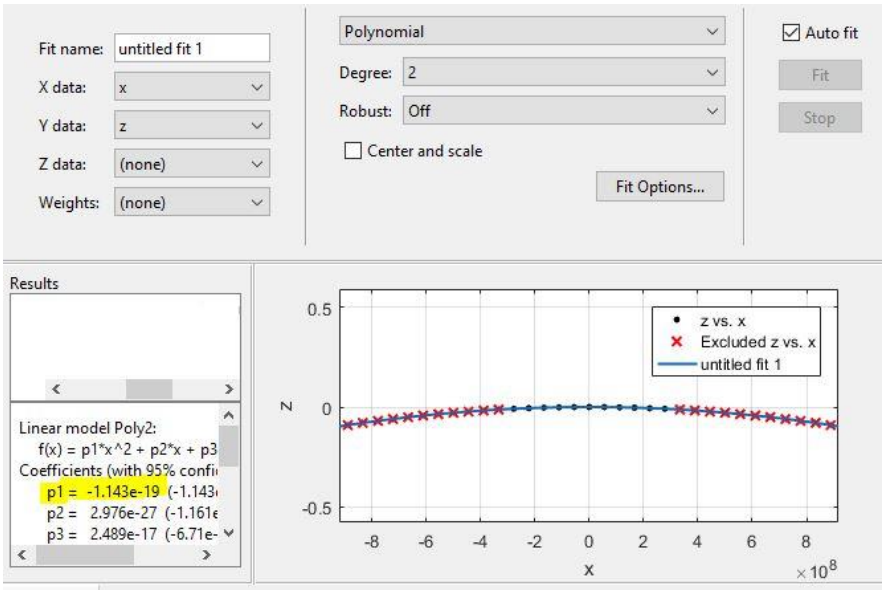

Fig: Curve fitting for heavy hole effective mass along [100] directions

Band struecture of Valence band of GaAs:

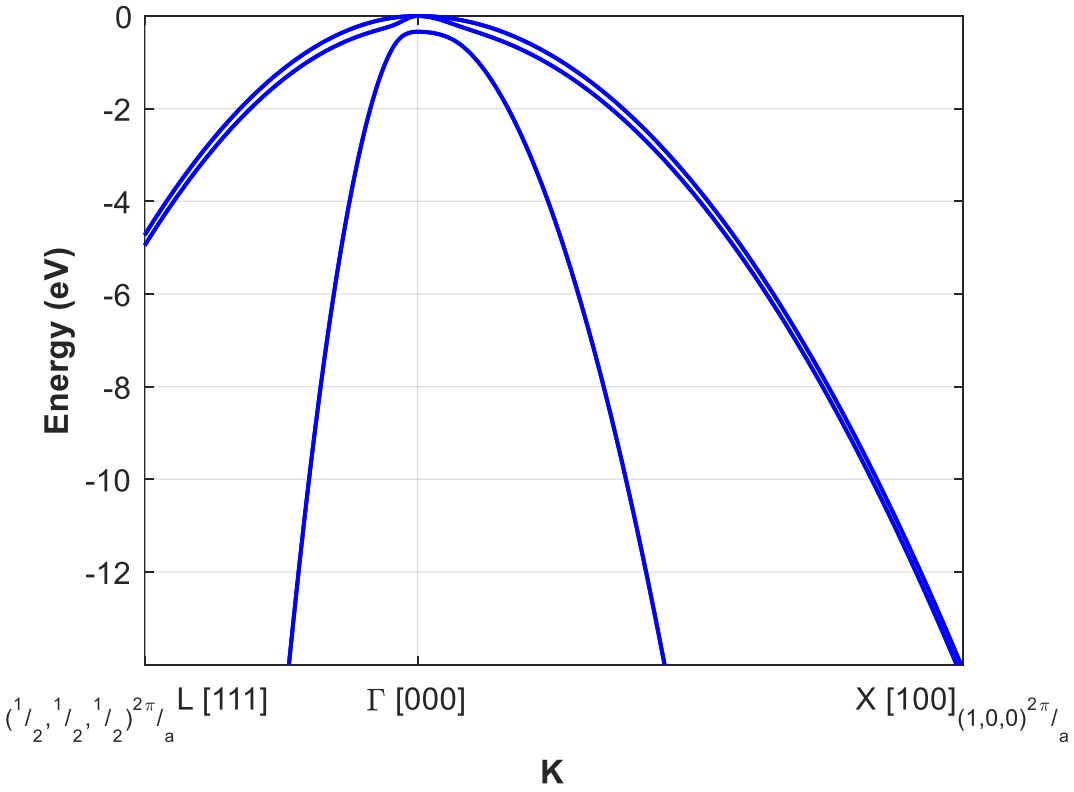

Fig: Band diagram along [100] and [111] directions

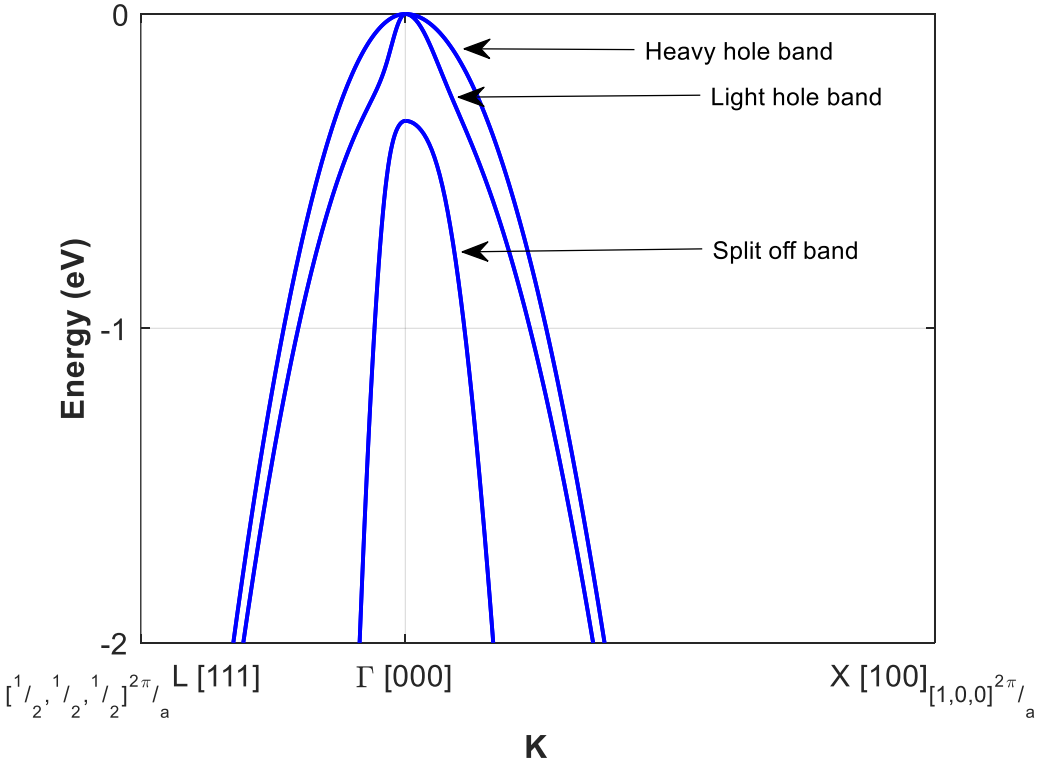

Fig: Zoomed view of band diagram along [100] and [111] directions

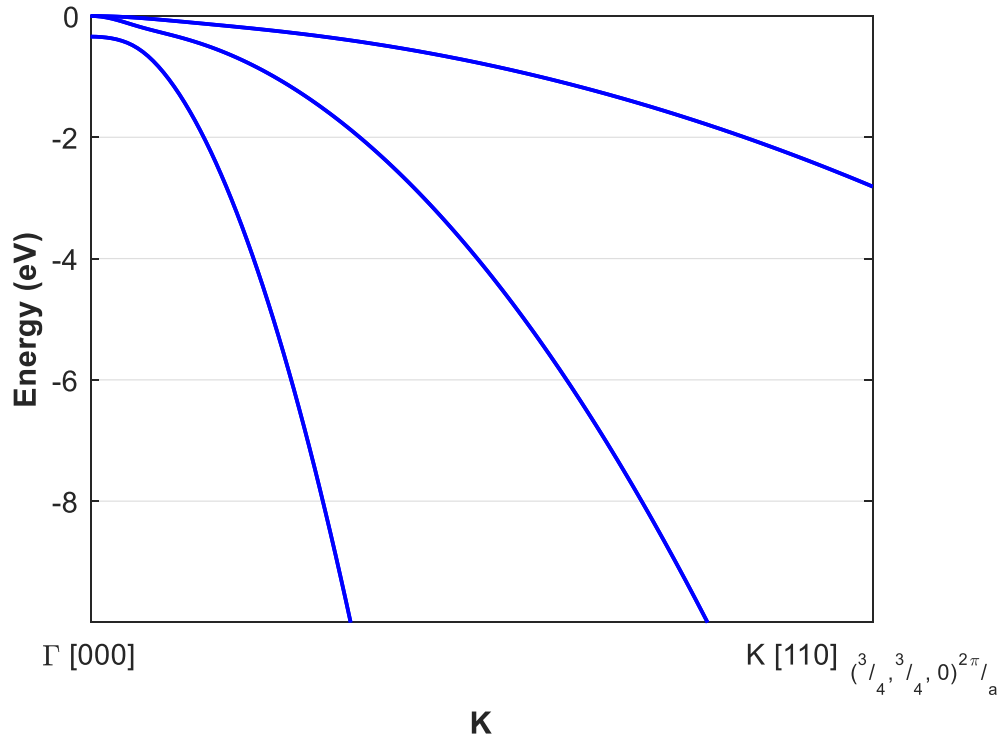

Fig: Band diagram along [110] direction

3.

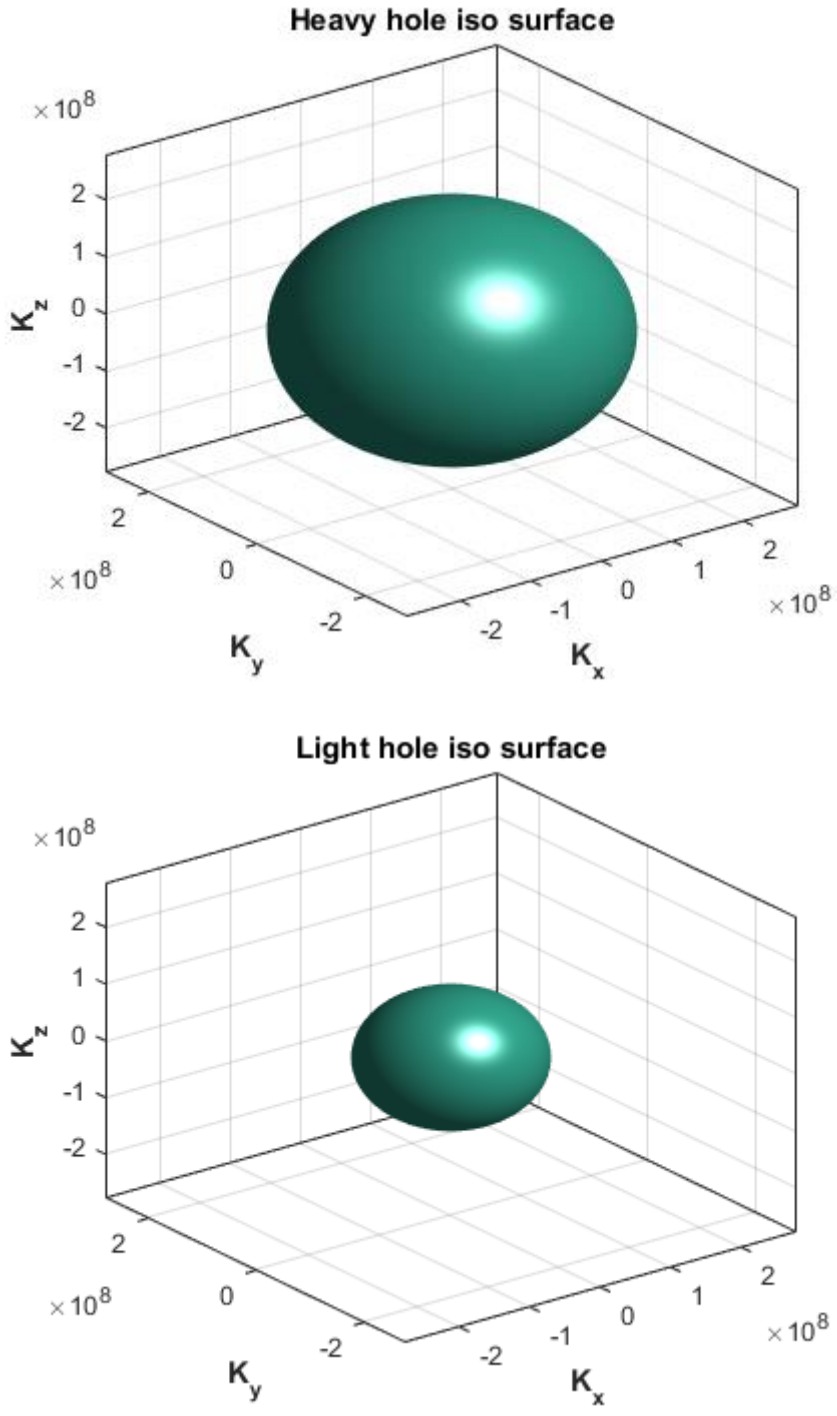

Fig: Energy isosurfaces for -0.005 eV

The top most point of the valence band of band structure is at Γ - point. The band structure is isotropic in nature i.e. the effective masses along longitudinal and transverse direction is same.

Thus the isosurfaces of heavy hole and light hole are spheres. They are calculated using the following equations:

$$E(K) = -\frac{\hbar^2}{2m_{hh}}\left[k_x^2 + k_y^2 + k_z^2\right] \quad \text{for heavy hole}$$

$$E(K) = -\frac{\hbar^2}{2m_{lh}}\left[k_x^2 + k_y^2 + k_z^2\right] \quad \text{for light hole}$$

The graphs plotted in the figure indicates the isosurface for -0.005 eV for both heavy hole and light hole where $m_{hh} = 0.333m_o$ and $m_{lh} = 0.0967m_o$. The sphere for light hole has smaller radius as it has less effective mass compared to that of heavy hole.

4. Density of states determined using stochastic approach

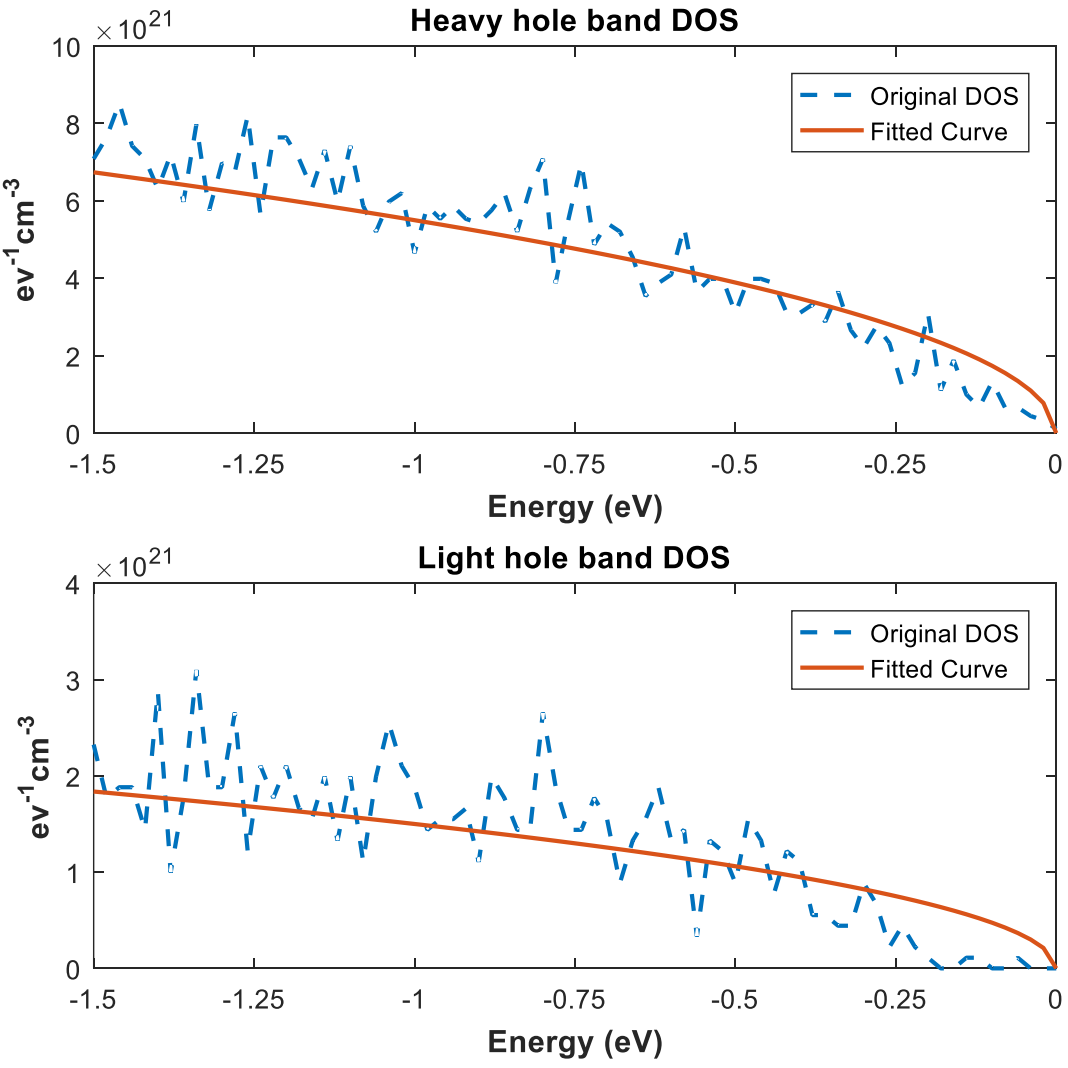

Fig: Density of states calculated using stochastic method

The density of states plots roughly varies as a square root of energy. For heavy hole band it is fitted to $DOS = 5.5\times10^{21}\sqrt{|E|}$ and for light hole band it is fitted to $DOS = 1.5\times10^{21}\sqrt{|E|}$

5. Energies at different k-points

K points	Heavy hole energy (eV)	Light hole energy (eV)	Split off band energy (eV)
(0.2, 0, 0)	-0.56477	-0.77887	-2.8368
(0.4, 0, 0)	-2.2591	-2.4827	-10.9599
(0.2, 0.2, 0)	-0.29025	-1.2533	-6.4772

Extra Question:

In deterministic method, firstly a k-point grid has been fixed and the energy range between 0 to -1.5eV is discretized. Then energy of the heavy hole band is calculated at all the fixed k-points of the chosen grid. Then those calculated energies obtained from solving hamiltonian matrix are compared with the discretized energy bins between the range 0 ~ -1.5 eV to find out in which energy bin they belong. The accuracy of this deterministic approach depends on the resolution i.e. the spacing between the k-points in the chosen grid. The denser the k-point grid the more accurate the result will be. From the following graph we can observe a good correlation between the DOS calculated by deterministic and stochastic approach.

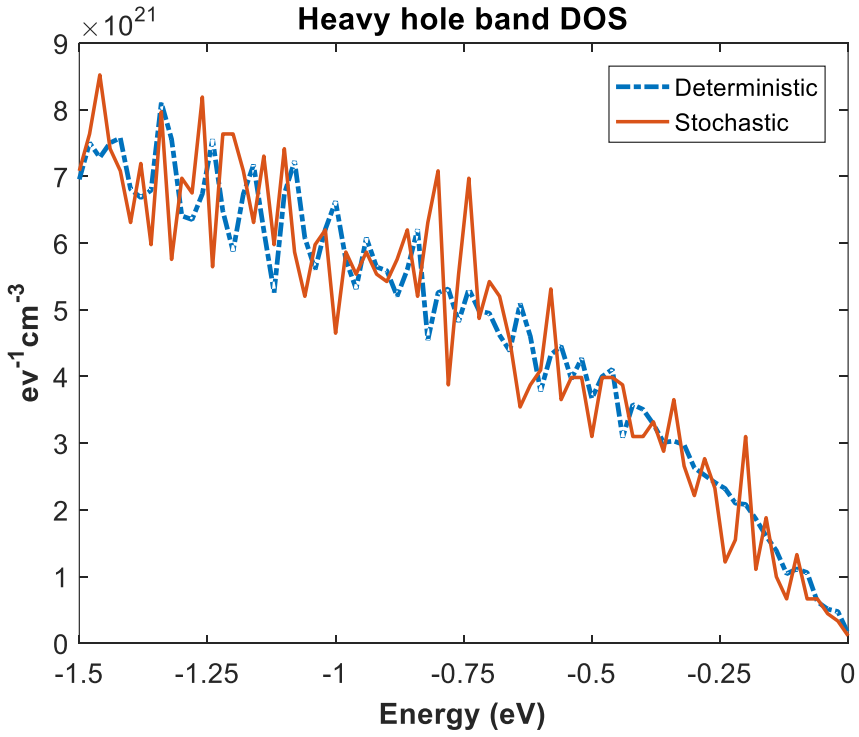

Fig: Comparison between deterministic and stochastic approach