1a)   The second partial differential operator can be written as,

$$\frac{d^2}{dx^2}\Psi_j = \frac{1}{a^2}\left(\Psi_{j-1} - 2\Psi_j + \Psi_{j+1}\right)$$

Hence,

$$-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\Psi_j = t\left(-\Psi_{j-1} + 2\Psi_j - \Psi_{j+1}\right)$$

1b)   Given that $\Psi(x) = \exp(ikx)$,

$$(E - U)\Psi = t\left[-2\cos(ka) + 2\right]\Psi$$
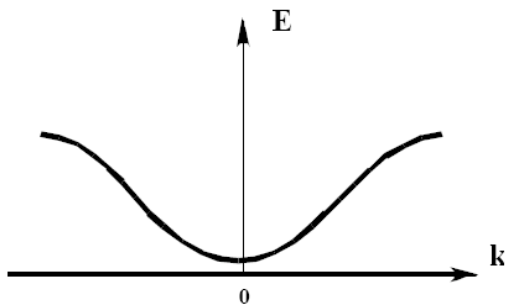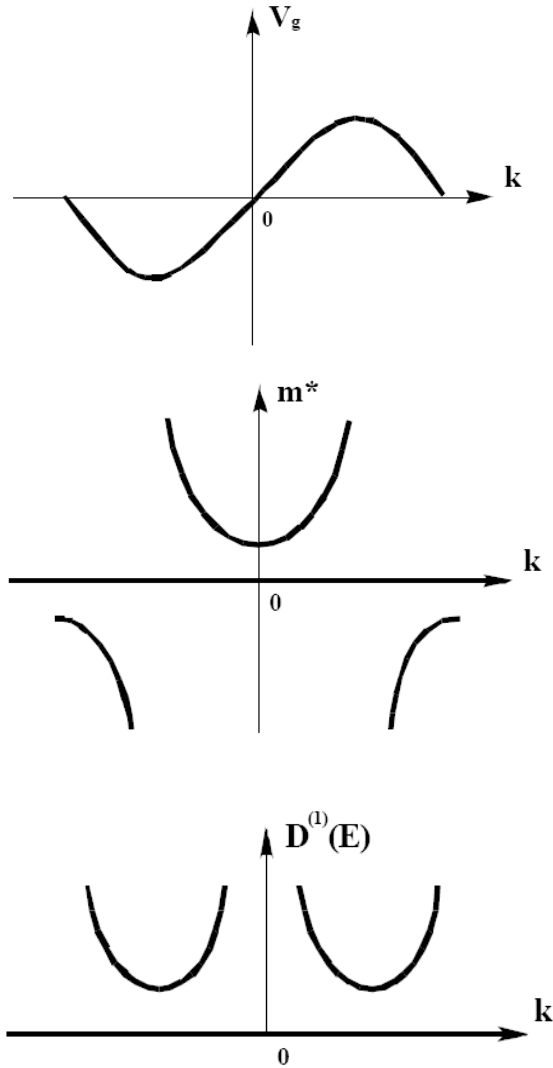$$E - U = 2t\left[1 - \cos(ka)\right]$$

When a is small,

$$E - U = 2t\left[\frac{k^2 a^2}{2}\right] = \frac{\hbar^2 k^2}{2m}$$

1c) $$v_G = \frac{1}{\hbar}\frac{\partial E}{\partial k} = \frac{2at}{\hbar}\sin(ka)$$

$$m = \hbar^2\left(\frac{\partial^2 E}{\partial k^2}\right)^{-1} = \frac{\hbar^2}{2a^2 t\cos(ka)}$$

$$DOS = \frac{\partial(2k)}{\partial E}\left(\frac{2}{2\pi}\right) = \frac{2}{\pi}\frac{\partial k}{\partial E} = \frac{1}{\pi a t\sin(ka)}$$

V_g

k

0

m^*

k

0

$D^{(1)}(E)$

k

0

1d)   When ka=0, velocity is zero and acceleration is positive
When ka=π/2, velocity is positive and maximum and acceleration is zero
When ka=π, velocity is zero and acceleration is negative

2a)   Eg is the difference between the lowest attainable conduction band and the highest attainable valence band. One deduces Eg = 1.42eV from Fig 3.13d. The Fig. 3.17 inset list Eg = 1.422eV for GaAs at 300K. The values are consistent.

2b)   The conduction band minimum and valence band maximum occurs at the same value of k in Fig 3.13d. This makes GaAs a direct semiconductor.

2c)   The curvature of the respective bands near k=0 is greatest for the conduction band and smallest for the heavy hole band. This would imply that m_e^* should be the smallest and m_{hh}^* the largest of the effective mass listed for GaAs in table

3.1.   This is indeed the case. The light hole band curvature is somewhat greater than that of the heavy hole band near k=0, and consistently $m_{hh}^* > m_{lh}^*$. However, the difference in curvature near k=0 between the two hole bands does not appear consistent. The split off band curvature is consistent with $m_{so}^* > m_{hh}^*$.

3a)   Dividing both sides of Eq. 3.47 by E-Ec yields

$$\frac{k_1^2}{\frac{2m_l^*}{\hbar^2}(E - E_c)} + \frac{k_2^2 + k_3^2}{\frac{2m_t^*}{\hbar^2}(E - E_c)} = 1$$

Hence

$$\alpha = \sqrt{\frac{2m_l^*}{\hbar^2}(E - E_c)}$$

$$\beta = \sqrt{\frac{2m_t^*}{\hbar^2}(E - E_c)}$$

Clearly,

$$\frac{\alpha}{\beta} = \left(\frac{m_l^*}{m_t^*}\right)^{0.5}$$

3b)   table 3.1 gives

$$\frac{m_l^*}{m_t^*} = \frac{1.588}{0.08152} = 19.48 \quad \text{for Ge}$$

$$\frac{m_l^*}{m_t^*} = \frac{0.9163}{0.1905} = 4.81 \quad \text{for Si}$$

We therefore expect,

$$\frac{\text{longitudinal axis length}}{\text{transverse axis length}} = \begin{cases} 4.41 \text{ for Ge} \\ 2.19 \text{ for Si} \end{cases}$$

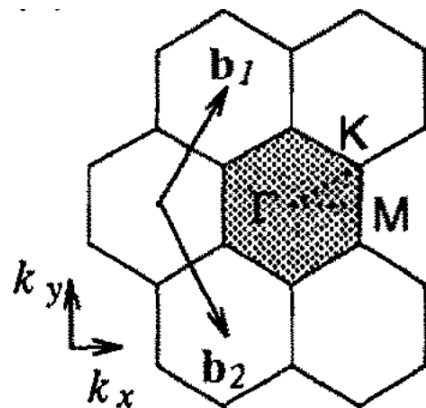Fig. 3.14 indeed shows a longitudinal/transverse axis length ratio of about 4:1 for Ge and about 2:1 or Si.

4a) $\vec{a}_1 \cdot (\vec{a}_2 \times \vec{a}_3) = \frac{3\sqrt{3}}{2}L^2$

$$\vec{b}_1 = \frac{4\pi}{3\sqrt{3}L}\begin{pmatrix} \sqrt{3}/2 \\ -3/2 \\ 0 \end{pmatrix} = \frac{2\pi}{L}\begin{pmatrix} 1/3 \\ -1/\sqrt{3} \\ 0 \end{pmatrix} \qquad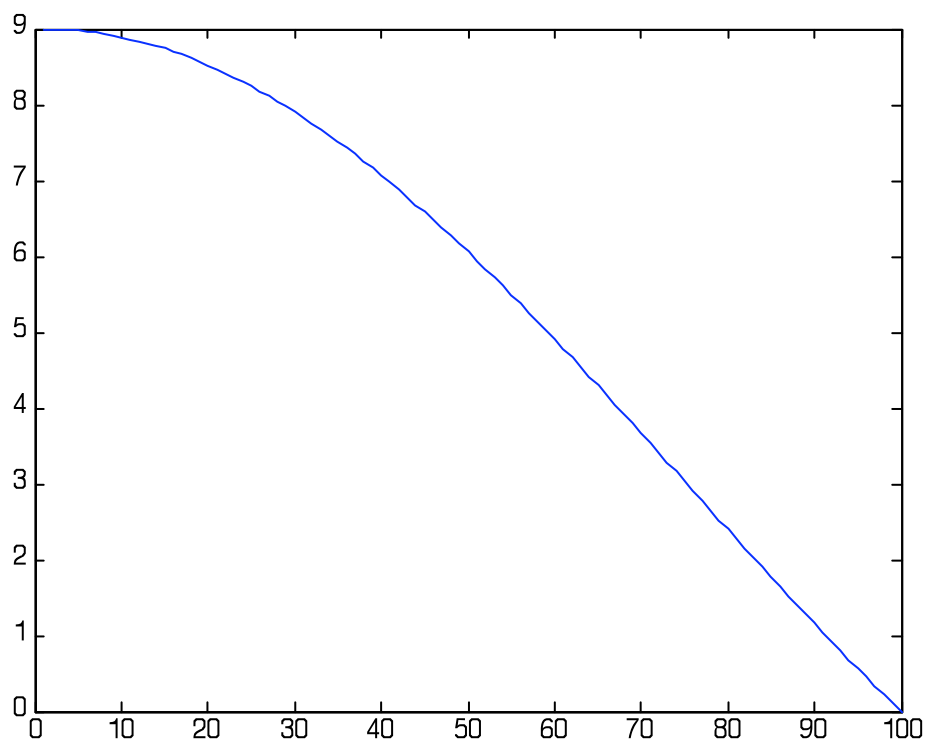 \vec{b}_2 = \frac{4\pi}{3\sqrt{3}L}\begin{pmatrix} \sqrt{3}/2 \\ 3/2 \\ 0 \end{pmatrix} = \frac{2\pi}{L}\begin{pmatrix} 1/3 \\ 1/\sqrt{3} \\ 0 \end{pmatrix}$$

4b)   One of the corner is

$$\frac{2\pi}{L}\begin{pmatrix} 1/3 \\ 1/3\sqrt{3} \\ 0 \end{pmatrix}$$

4c)   effective mass is undefined. Velocity is about 1E6 m/s

4d)   the density of states for graphene:

$$DOS = \frac{\partial}{\partial E}\left(\frac{\pi k^2 2}{4\pi^2}\right) = \frac{\partial}{\partial E}\left(\frac{k^2}{2\pi}\right) = \frac{E}{\pi \hbar^2 v^2}$$

the density of states for semicon:

$$DOS = \frac{\partial}{\partial E}\left(\frac{\pi k^2 2}{4\pi^2}\right) = \frac{\partial}{\partial E}\left(\frac{k^2}{2\pi}\right) = \frac{m}{\pi \hbar^2}$$

the 0T electron density for graphene:

$$n = \int_0^E \frac{E}{\pi \hbar^2 v^2} dE = \frac{E^2}{2\pi \hbar^2 v^2}$$

the 0T electron density for semicon:

$$n = \frac{mE}{\pi \hbar^2}$$

In general we should have $n = \int_0^E D(E) f(E) dE$. f(E) is the Fermi Dirac distribution. For semiconductor, only T dependent near the band edge. Not T dependent at high energy, since area under Fermi Dirac function is unchanged with T. For graphene, T dependent near band edge, but weak T dependent at high energy since D(E) for graphene is not constant.

6a)   The crystal structure is zinc-blende. Zinc blende has 2 inter-penetrating fcc lattices

6b)   There are 2 atoms in the primitive unit cell of GaAs

6c)   Conduction Band energies at Gamma, X, L valleys are 1.42, 1.9, and 1.71 (all values in eV).

6d)   The three bands are classified as heavy hole, light hole, and split off bands. They form the valence bands.

6e)   The split is due to spin orbit coupling. It is equal to 0.343 eV for our case.

6f)   The effective masses in the L valley are higher than the gamma valley.

6g)   At high electric fields, the conduction electrons in GaAs are transported to the L valley. As noted in the previous question, the L valley has a higher effective mass; consequently the conductivity decreases with increasing electric field leading to NDR.

6h)   The Gunn diode uses the principle of NDR. It is used for the generation of microwaves.

To read more about the NDR phenomenon in GaAs, please consult "Fundamentals of Semiconductor" –Yu and Cardona; 3rd edition, Springer. Pg 228-230.
Another good book is Theory of modern electronic semiconductor devices By Kevin F. Brennan, April S. Brown Pg 195-232.