\[ E_n = 0.7521, \text{ so } E_{\text{cont}} = E - E_n = 1 - 0.7521 = 0.2479. \text{ Using } E = \hbar \omega, \]
\[ 0.2479 = \frac{\hbar^2}{|q_e|2m_e} k_z^2 \to k_z = \sqrt{\frac{0.2479|q_e|2m_e}{\hbar^2}} = 2.551 \times 10^6 \]

(144)

\[ \frac{\hbar^2}{2m_e} k_z^2 = \hbar \omega \]

\[(v_g)_z = \frac{\partial \omega}{\partial k_z} = \frac{\hbar}{2m_e} 2k_z = \frac{\hbar}{2m_e} (2.551 \times 10^6) = 2.953 \times 10^5 \text{ m/s}. \]

4.22. A 3 eV electron is to be confined in a square quantum dot of side \( L \). What should \( L \) be in order for the electron’s energy levels to be well-quantized?

Solution: From (2.14),
\[ \lambda_e = \frac{h}{p} = \frac{h}{m_ev} = \frac{h}{m_e \sqrt{\frac{2E}{m_e}}} = \frac{h}{m_e \sqrt{\frac{2q_e}{m_e}}} = 0.708 \text{ nm}, \]

(145)

and we need \( L \leq \lambda_e \).

5 Problems Chapter 5: Electrons Subject to a Periodic Potential – Band Theory of Solids

5.1. To gain an appreciation of the important role of surface effects at the nanoscale, consider building up a material out of bcc unit cells. (See Section 5.1). For one bcc cube, there would be 9 atoms, 8 on the outside and one interior, as depicted on p. 134. If we constrain ourselves to only consider cubes of material, the next largest cube would consist of 8 bcc unit cells, and so on. If one unit cell is 0.5 nm, how long should the material’s side be in order for there to be more interior atoms than surface atoms?

Solution:

<table>
<thead>
<tr>
<th># unit cells in the cube</th>
<th>Surface Atoms</th>
<th>Interior Atoms</th>
<th>Ratio (S/I)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>8</td>
<td>1</td>
<td>8</td>
</tr>
<tr>
<td>(2^3 = 8)</td>
<td>26</td>
<td>9</td>
<td>2.9</td>
</tr>
<tr>
<td>(3^3 = 27)</td>
<td>56</td>
<td>35</td>
<td>1.6</td>
</tr>
<tr>
<td>(4^3 = 64)</td>
<td>98</td>
<td>91</td>
<td>1.1</td>
</tr>
<tr>
<td>(5^3 = 125)</td>
<td>152</td>
<td>189</td>
<td>0.8</td>
</tr>
</tbody>
</table>

so that we need \(5^3\) unit cells, leading to a material cube having side length \(5 \times 0.5 = 2.5 \text{ nm}\).

5.2. Consider the Kronig-Penney model of a material with \( a_1 = a_2 = 5 \text{ Å} \) and \( V_0 = 0.5 \text{ eV}\). Determine numerically the starting and ending energies of the first allowed band.

Solution: From
\[ \cos kT = \cos (\alpha a) \cosh (b\delta) - \frac{\alpha^2 - \beta^2}{2\alpha\delta} \sin (\alpha a) \sinh (b\delta), \]

(146)

if \(0 < E < V_0\), and
\[ \cos kT = \cos (\alpha a) \cos (b\beta) - \frac{\alpha^2 + \beta^2}{2\alpha\beta} \sin (\alpha a) \sin (b\beta), \]

(147)

if \(E > V_0\). Then, for \(0 < E < V_0\) the plot is Band edge energy occurs when \(\cos kT\) is \(\pm 1\). It is found numerically that \(\cos kT = -1\) when \(E = 0.459\), \(\cos kT = 0\) when \(E = 0.300\), and \(\cos kT = 1\) when \(E = 0.217\). Therefore, the band edges are at \(E = 0.217 \text{ eV}\) and \(E = 0.459 \text{ eV}\).

5.3. Use the equation of motion (5.34) to show that the period of Bloch oscillation for a one-dimensional crystal having lattice period \(a\) is
\[ \tau = \frac{\hbar}{e\mathcal{E}a}. \]

(148)
Solution: Use
\[ \hbar \frac{dk}{dt} = -e E, \]  
and assume that \( \tau \) is the time required for the electron to accelerate across the full Brillouin zone. Then,
\[ \hbar \int_0^{\tau/2} \frac{dk}{dt} dt = - \int_0^{\tau/2} e E dt \]
\[ \hbar \left( \frac{\tau}{2} - k(0) \right) = -e E \frac{\tau}{2} \]
\[ \hbar \left( \frac{\pi}{a} - 0 \right) = -e E \frac{\tau}{2} \]
\[ \tau = \frac{\hbar}{e E a}. \]

5.4. Determine the probability current density (A/m) from (3.187) for the Bloch wavefunction
\[ \psi(x) = u(x) e^{ikx} e^{-i\omega t}, \]  
where \( u \) is a time-independent periodic function having the period of the lattice,
\[ u(x) = u(x + a). \]

Solution:
\[ J(r, t) = \frac{-i\hbar}{2m} \left( \Psi^*(r, t) \nabla \Psi(r, t) - \Psi(r, t) \nabla \Psi^*(r, t) \right) \]
\[ = \frac{-i\hbar}{2m} \left( u(x) e^{-ikx} e^{i\omega t} \nabla (u(x) e^{ikx} e^{-i\omega t}) - u(x) e^{ikx} e^{-i\omega t} \nabla (u(x) e^{-ikx} e^{i\omega t}) \right) \]
\[ = \frac{\hbar}{2m} \left( u(x) e^{-ikx} e^{i\omega t} \frac{d}{dx} (u(x) e^{ikx} e^{-i\omega t}) - u(x) e^{ikx} e^{-i\omega t} \frac{d}{dx} (u(x) e^{-ikx} e^{i\omega t}) \right) \]
\[ = \frac{\hbar}{2m} \left( (u^2 ik + u'u) - (-u^2 ik + u'u) \right) \]
\[ = \frac{\hbar}{2m} (2u^2 ik) = \frac{\hbar k}{m} u^2 = \frac{p}{m} u^2. \]

5.5. If an energy-wavevector relationship for a particle of mass \( m \) has the form
\[ E = \frac{\hbar^2 k^2}{3m}, \]  
determine the effective mass. (Use (5.29)).

Solution:
\[ m^* = \hbar^2 \left( \frac{\partial^2 E}{\partial k^2} \right)^{-1} = \hbar^2 \left( \frac{\partial^2 \left( \frac{\hbar^2 k^2}{3m} \right)}{\partial k^2} \right)^{-1} = \frac{3}{2} m. \]

5.6. If the energy-wavenumber relationship for an electron in some material is
\[ E = \frac{\hbar^2}{2m} \cos(k), \]
determine the effective mass and the group velocity. (Use (5.29).) Describe the motion (velocity, direction, etc.) of an electron when a d.c. (constant) electric field is applied to the material, such that the electric field vector points right to left (e.g., an electron in free space would then accelerate towards the right). In particular, describe the motion as \( k \) varies from 0 to \( 2\pi \). Assume that the electron does not scatter from anything.
Solution:

\[ m^* = h^2 \left( \frac{\partial^2 E}{\partial k^2} \right)^{-1} = h^2 \left( \frac{\partial^2 \left( \frac{\hbar^2}{2m} \cos (k) \right)}{\partial k^2} \right)^{-1} = -\frac{2m}{\cos k} \] (156)

\[ v_g = \frac{1}{\hbar} \frac{\partial E}{\partial k} = \frac{1}{\hbar} \frac{\partial}{\partial k} \left( \frac{\hbar^2}{2m} \cos (k) \right) = -\frac{1}{2m} \frac{\hbar}{E} \sin k \] (157)

For small positive \( k \) values the electron moves in the direction of the field (to the left), and as \( k \) increases through positive value from \( k = 0 \) to \( k = \pi/2 \), the electron increases its velocity and mass. At \( k = \pi/2 \), velocity is maximum and the effective mass is infinite. As \( k \) changes from \( \pi/2 \) to \( \pi \), the velocity decreases, as does the effective mass. At \( k = \pi \), the velocity is zero. Then, as \( k \) increases further, the electron reverses direction, and it’s velocity increases again, reaching a maximum at \( k = 3\pi/2 \), then decreasing till \( k = 2\pi \).

5.7. If the energy-wavenumber relationship for an electron in some material is

\[ E = E_0 + 2A \cos (ka), \] (158)

determine the electron’s position as a function of time. Ignore scattering.

**Solution:** The solution of the equation of motion (ignoring scattering) is (5.36),

\[ k(t) = k(0) + \frac{q_e E}{\hbar} t. \] (159)

Velocity is given as

\[ v_g(k(t)) = \frac{1}{\hbar} \frac{\partial E(k(t))}{\partial k} = \frac{2Aa}{\hbar} \sin (k(t)a) \] (160)

\[ = -\frac{2Aa}{\hbar} \sin \left( \frac{q_e E a}{\hbar} t \right) \] (161)

and position can be determined from the relationship \( v = dx(t)/dt \) as

\[ x(t) = \int_0^t v_g(t) \, dt = -\int_0^t \frac{2Aa}{\hbar} \sin \left( \frac{q_e E a}{\hbar} t \right) \, dt \] (162)

\[ = \frac{2A}{q_e E a} \left( \cos \left( \frac{q_e E a}{\hbar} t \right) - 1 \right), \] (163)

and therefore the electron Bloch oscillates in time.

5.8. Consider an electron in a perfectly periodic lattice, wherein the energy-wavenumber relationship in the first Brillouin zone is

\[ E = \frac{\hbar^2 k^2}{5m_e}, \]

where \( m_e \) is the mass of an electron in free space. Write down the time-independent effective mass Schrödinger’s equation for one electron in the first Brillouin zone, ignoring all interactions except between the electron and the lattice. Define all terms in Schrödinger’s equation.

**Solution:**

\[ m^* = h^2 \left( \frac{\partial^2 E}{\partial k^2} \right)^{-1} = \frac{\hbar^2}{\frac{\hbar^2}{5m_e}} \left( \frac{\partial^2}{\partial k^2} \right)^{-1} = \frac{5}{2}m_e, \] (164)

and so Schrödinger’s equation is

\[ \left( -\frac{\hbar^2}{2m^*} \frac{d^2}{dx^2} \right) \psi(x) = E \psi(x) \] (165)

where \( m^* \) is the effective mass, \( \hbar \) is the reduced Planck’s constant, and \( E \) is the energy (\( V = 0 \) since there is no potential energy term; potential energy is accounted for by the effective mass).
5.9. Assume that a constant electric field of strength $E = -1\text{ kV/m}$ is applied to a material at $t = 0$, and that no scattering occurs.

(a) Solve the equation of motion (5.34) to determine the wavevector value at $t = 1, 3, 7,$ and $10\text{ ns}$.
(b) Assuming that the period of the lattice is $a = 0.5\text{ nm}$, determine in which Brillouin zone the wavevector is in at each time. If the wavevector lies outside the first Brillouin zone, map it into an equivalent place in the first zone.

**Solution:**

(a) The solution of the equation of motion is 

$$k(t) = \frac{q_e E}{h} t,$$  

assuming $k(0) = 0$. Then $k(1\text{ ns}) = 1.52 \times 10^9\text{ m}^{-1}$, $k(3\text{ ns}) = 4.56 \times 10^9\text{ m}^{-1}$, $k(7\text{ ns}) = 1.06 \times 10^{10}\text{ m}^{-1}$, and $k(10\text{ ns}) = 1.52 \times 10^{10}\text{ m}^{-1}$.

(b) Brillouin zone boundaries occur at $k_n = \pm n\pi/a$, where $a$ is the period and $n = 1, 2, 3, \ldots$. Thus, $k_1 = \pm 6.28 \times 10^9\text{ m}^{-1}$, $k_2 = \pm 1.26 \times 10^{10}\text{ m}^{-1}$, $k_3 = \pm 1.89 \times 10^{10}\text{ m}^{-1}$, etc. Thus, $k$ is in the first zone for $t = 1$ and $3$, the second zone for $t = 7$, and the third zone for $t = 10$. For higher zones, subtracting $2\pi/a$ leads to the equivalent point in the first zone.

<table>
<thead>
<tr>
<th>$t$ (ns)</th>
<th>$k(t)$ (m$^{-1}$)</th>
<th>zone</th>
<th>equiv. point in 1st zone</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>$1.52 \times 10^9$</td>
<td>1st</td>
<td>–</td>
</tr>
<tr>
<td>3</td>
<td>$4.56 \times 10^9$</td>
<td>1st</td>
<td>–</td>
</tr>
<tr>
<td>7</td>
<td>$1.06 \times 10^{10}$</td>
<td>2nd</td>
<td>$-1.966 \times 10^9$</td>
</tr>
<tr>
<td>10</td>
<td>$1.52 \times 10^{10}$</td>
<td>3rd</td>
<td>$2.63 \times 10^9$</td>
</tr>
</tbody>
</table>

5.10. Using the hydrogen model for ionization energy, determine the donor ionization energy for GaAs ($m_e^* = 0.067m_e$, $\varepsilon_e = 13.1$).

**Solution:**

$$\Delta E_d = \frac{0.067m_e q_e^2}{|q_e| 8 (13.1)^2 \varepsilon_e^2 h^2} = 5.32 \text{ meV}. \quad (167)$$

This compares well with measured values.

5.11. Determine the maximum kinetic energy that can be observed for emitted electrons when photons having $\lambda = 232\text{ nm}$ are incident on a metal surface with work function $5\text{ eV}$.

**Solution:**

$$E = \hbar \omega = \hbar \left( \frac{2\pi c}{\lambda} \right) = \hbar \left( \frac{2\pi c}{232 \times 10^{-9}} \right) = 8.568 \times 10^{-19}\text{ J}$$

$$= 5.347 \text{ eV}$$

So, the maximum kinetic energy is

$$E - e\phi = 0.347 \text{ eV}. \quad (169)$$

5.12. Photons are incident on silver, which has a work function $e\phi = 4.8\text{ eV}$. The emitted electrons have a maximum velocity of $9 \times 10^5\text{ m/s}$. What is the wavelength of the incident light?

**Solution:**

$$E_{KE} = \frac{1}{2} m_e v^2 = \frac{1}{2} |q_e| m_e \left( 9 \times 10^5 \right)^2 = 2.303 \text{ eV} \quad (170)$$

$$E = \hbar \omega = e\phi + E_K = 4.8 + 2.303 = 7.103 \text{ eV},$$

$$\lambda = \frac{hc}{E} = \frac{hc}{7.103 |q_e|} = 174.67\text{ nm}. \quad (172)$$
5.13. In the band theory of solids, there are an infinite number of bands. If, at \( T = 0 \) K, the uppermost band to contain electrons is partially filled, and the gap between that band and the next lowest band is 0.8 eV, is the material a metal, an insulator, or a semiconductor?

**Solution:** Metal

5.14. In the band theory of solids, if, at \( T = 0 \) K, the uppermost band to have electrons is completely filled, and the gap between that band and the next lowest band is 8 eV, is the material a metal, an insulator, or a semiconductor? What if the gap is 0.8 eV.

**Solution:** Insulator. What if the gap is 0.8 eV. **Solution:** Semiconductor

5.15. Describe in what sense an insulator with a finite band gap cannot be a perfect insulator.

**Solution:** As long as the band gap is finite, an electron can be elevated to the conduction band, resulting in conduction.

5.16. Draw relatively complete energy band diagrams (in both real-space and momentum space) for a \( p \)-type indirect bandgap semiconductor.

5.17. For an intrinsic direct bandgap semiconductor having \( E_g = 1.72 \text{ eV} \), determine the required wavelength of a photon that could elevate an electron from the top of the valance band to the bottom of the conduction band. Draw the resulting transition on both types of energy band diagrams (i.e., energy-position and energy-wavenumber diagrams).

**Solution:**

\[
\hbar \omega = E_g = 1.72 \text{ eV},
\]

\[
k = \frac{2\pi}{\lambda} = \frac{\omega}{c} \rightarrow \lambda = \frac{2\pi c}{\omega} = \frac{2\pi c}{E_g/\hbar} = 721.3 \text{ nm}.
\]

5.18. Determine the required phonon energy and wavenumber to elevate an electron from the top of the valance band to the bottom of the conduction band in an indirect bandgap semiconductor. Assume that \( E_g = 1.12 \text{ eV} \), the photon’s energy is \( E_{pt} = 0.92 \text{ eV} \), and that the top of the valance band occurs at \( k = 0 \), whereas the bottom of the conduction band occurs at \( k = k_a \).

\[
E_g - E_{pt} = E_{pn} = 0.20 \text{ eV}
\]

\[
k_{pn} = k_a.
\]

5.19. Calculate the wavelength and energy of the following transitions of an electron in a hydrogen atom. Assuming that energy is released as a photon, using Table 3, on p. 4 classify the emitted light (e.g., X-ray, IR, etc.).

(a) \( n = 2 \to n = 1 \)

**Solution:** From

\[
E_n = -13.6 \frac{1}{n^2},
\]

and so

\[
\Delta E = -13.6 \left( \frac{1}{2^2} - \frac{1}{1^2} \right) = 10.2 \text{ eV},
\]

\[
\lambda = \frac{\hbar c}{E} = \frac{\hbar c}{10.2 |q_e|} = 121.6 \text{ nm, between visible and UV}
\]

(b) \( n = 5 \to n = 4 \)

\[
\Delta E = -13.6 \left( \frac{1}{5^2} - \frac{1}{4^2} \right) = 0.306 \text{ eV},
\]

\[
\lambda = \frac{\hbar c}{E} = \frac{\hbar c}{0.306 |q_e|} = 4054.5 \text{ nm, far-infrared}
\]
5.20. Excitons were introduced in Section 5.4.5 to account for the fact that sometimes when an electron is elevated from the valance band to the conduction band, the resulting electron and hole can be bound together by their mutual Coulomb attraction. Excitonic energy levels are located just below the band gap, since the usual energy to create a free electron and hole, \(E_g\), is lessened by the binding energy of the exciton. Thus, transitions can occur at

\[
E = E_g - \frac{m^*}{m_e \varepsilon^2_r} 13.6 \text{ eV}
\]

where \(E_g\) is in electron volts\(^1\).

(a) For GaAs, determine the required photon energy to create an exciton. For \(m^*\) use the average of the heavy and light hole masses.

**Solution:** Using \(m^* = 0.0502 \text{me}, \varepsilon_r = 13.3, \text{ and } E_g = 1.43 \text{ eV, we find that}

\[
E = E_g - \frac{m^*}{m_e \varepsilon^2_r} 13.6 \text{ eV}
\]

\[
= 1.43 - \frac{0.0502}{(13.3)^2} 13.6 \text{ eV}
\]

\[
= 1.426 \text{ eV}.
\]

(b) The application of a d.c. electric field tends to separate the electron and the hole. Using Coulomb’s law, show that the magnitude of the electric field between the electron and the hole is

\[
|\mathcal{E}| = \left(\frac{m^*}{m_e}\right)^2 \frac{2}{\varepsilon^3_r |q_e|} \frac{R_Y}{a_0}.
\]

\(^1\)Really, the quantity 13.6 should be replaced by 13.6/\(n^2\), where \(n\) is the energy level of the exciton. Here we consider the lowest level exciton \((n = 1)\), which is dominant.
Solution: The electric field due to a charge $q$ in a medium characterized by $\varepsilon_r$ is

$$E = \hat{r} \frac{q}{4\pi \varepsilon_r \varepsilon_0 r^2} = \hat{r} |\varepsilon|,$$

(187)

where $\hat{r}$ is a unit vector that points radially outward from the charge, and $r$ is the radial distance away from the charge. Making the substitutions $q = q_e$ and $r = a_e$ leads to

$$|\varepsilon| = \frac{|q_e|}{4\pi \varepsilon_r \varepsilon_0 a_e^2} = \left( \frac{m_r^*}{m_e} \right)^2 \frac{|q_e|}{4\pi \varepsilon_r \varepsilon_0 a_e^2}$$

(188)

$$= \left( \frac{m_r^*}{m_e} \right)^2 \frac{m_e |q_e|}{4\pi \varepsilon_r \varepsilon_0} = \left( \frac{2 R_Y}{|q_e|} \right) \frac{1}{\varepsilon_r^2 a_0}$$

(189)

$$= \left( \frac{m_r^*}{m_e} \right)^2 \frac{2 R_Y}{\varepsilon_r^2 |q_e| a_0}$$

(190)

(c) For GaAs, determine $|\varepsilon|$ from (5.79). Determine the magnitude of an electric field that would break apart the exciton.

Solution:

$$|\varepsilon| = \left( \frac{m_r^*}{m_e} \right)^2 \frac{2 R_Y}{\varepsilon_r^2 |q_e| a_0}$$

(191)

$$= (0.0502)^2 \frac{2 R_Y}{(13.3)^2 |q_e| a_0} \frac{13.6 |q_e|}{0.053 \times 10^{-5}} = 5.5 \times 10^5 \text{ V/m.}$$

(192)

An applied electric field with a magnitude greater than $|\varepsilon|$ can break apart the exciton.

5.21. The $E - k$ relationship for graphene is given by (5.62). The Fermi energy for graphene is $E_F = 0$, and the first Brillouin zone forms a hexagon (as shown in Fig. 5.35), the six corners of which correspond to $E = E_F = 0$. The six corners of the first Brillouin zone at located at

$$k_x = \pm \frac{2\pi}{\sqrt{3}a}, \quad k_y = \pm \frac{2\pi}{3a},$$

(193)

and

$$k_x = 0, \quad k_y = \pm \frac{4\pi}{3a}.$$  

(194)

(a) Verify that at these points, $E = E_F = 0$.

Solution:

$$E(k_x, k_y) = \pm \gamma_0 \sqrt{1 + 4 \cos \left( \frac{\sqrt{3}k_x a}{2} \right) \cos \left( \frac{k_y a}{2} \right) + 4 \cos^2 \left( \frac{k_y a}{2} \right)},$$

$$E \left( 0, \pm \frac{4\pi}{3a} \right) = \pm \gamma_0 \sqrt{1 + 4 \cos \left( \pm \frac{4\pi}{3a} \cdot \frac{a}{2} \right) + 4 \cos^2 \left( \pm \frac{4\pi}{3a} \cdot \frac{a}{2} \right)}$$

$$= \pm \gamma_0 \sqrt{1 + 4 \cos \left( \frac{2\pi}{3} \right) + 4 \cos^2 \left( \frac{2\pi}{3} \right)} = 0$$

$$E(k_x, k_y) = \pm \gamma_0 \sqrt{1 + 4 \cos \left( \frac{\sqrt{3}k_x a}{2} \right) \cos \left( \frac{k_y a}{2} \right) + 4 \cos^2 \left( \frac{k_y a}{2} \right)},$$

$$E \left( \pm \frac{2\pi}{\sqrt{3}a}, \pm \frac{2\pi}{3a} \right) = \pm \gamma_0 \sqrt{1 + 4 \cos \left( \pm \frac{2\pi}{\sqrt{3}a} \cdot \frac{a}{2} \right) \cos \left( \pm \frac{2\pi}{3a} \cdot \frac{a}{2} \right) + 4 \cos^2 \left( \pm \frac{2\pi}{3a} \cdot \frac{a}{2} \right)}$$

$$= \pm \gamma_0 \sqrt{1 + 4 \cos \left( \frac{\pi}{3} \right) + 4 \cos^2 \left( \frac{\pi}{3} \right)} = 0.$$
(b) At the six corners of the first Brillouin zone, \( |k| = 4\pi/3a \). Make a two-dimensional plot of the \( E - k \) relationship for \( k_x, k_y \) extending a bit past \( |k| \). Verify that the bonding and antibonding bands touch at the six points of the first Brillouin zone hexagon, showing that graphene is a semi-metal (sometimes called a zero bandgap semiconductor). Also make a one-dimensional plot of \( E(0, k_y) \) for \( -|k| \leq k_y \leq |k| \), showing that the bands touch at \( E = 0 \) at \( k_y = \pm 4\pi/3a \).

Solution:
Using (5.62), since \( a = \sqrt{3}(0.142 \text{ nm}) = 0.246 \text{ nm} \), \( |k| = 4\pi/3a = 17 \text{ nm}^{-1} \). Thus,

\[
E(0, k_y) = \pm \gamma_0 \sqrt{1 + 4 \cos \left(\frac{k_y a}{2}\right) + 4 \cos^2\left(\frac{k_y a}{2}\right)}
\]

\[
= \pm 2.5 \sqrt{1 + 4 \cos \left(\frac{k_y 0.246}{2}\right) + 4 \cos^2\left(\frac{k_y 0.246}{2}\right)}
\]

we have

where the vertical scale is in eV and the horizontal scale is in nm\(^{-1}\).
5.22. What is the radius of a (19, 0) carbon nanotube? Repeat for a (10, 10) nanotube. Consider a \((n, 0)\) zigzag carbon nanotube that has radius 0.3523 nm. What is the value of the index \(n\)?

**Solution:** The CN’s radius is

\[
r = \frac{\sqrt{3}}{2\pi} b \sqrt{n^2 + nm + m^2},
\]

where \(b = 0.142\) nm. Therefore,

\[
r_{(19,0)} = \frac{\sqrt{3}}{2\pi} (0.142 \times 10^{-9}) \sqrt{19^2} = 0.7437 \text{ nm}
\]

\[
r_{(10,10)} = \frac{\sqrt{3}}{2\pi} (0.142 \times 10^{-9}) \sqrt{10^2 + (10)(10) + 10^2} = 0.678 \text{ nm}.
\]

For \((n, 0)\),

\[
n = \frac{2\pi a}{\sqrt{3} b} = \frac{2\pi (0.3523 \times 10^{-9})}{\sqrt{3} (0.142 \times 10^{-9})} = 9.
\]

5.23. Since carbon nanotubes are only periodic along their axis, the transverse wavenumber becomes quantized by the finite circumference of the tube. Derive (5.66) and (5.67) by enforcing the condition that an integer number \(q\) of transverse wavelengths must fit around the tube \((k_\perp = 2\pi/\lambda_\perp)\).

**Solution:** For the armchair tube \((m = n)\), tube radius is \(r = 3nb/2\pi\). Thus,

\[
q\lambda_\perp = 2\pi r = 2\pi \frac{3nb}{2\pi} = 3nb
\]

\[
k_\perp = k_{x,q} = \frac{2\pi q}{\lambda_\perp} = \frac{2\pi q}{n3b}, \quad q = 1, 2, ..., 2n.
\]

For zigzag tubes, \((n = 0)\), \(r = \sqrt{3}nb/2\pi\), and

\[
q\lambda_\perp = 2\pi r = 2\pi \frac{\sqrt{3}nb}{2\pi} = \sqrt{3}nb
\]

\[
k_\perp = k_{y,q} = \frac{2\pi q}{\lambda_\perp} = \frac{2\pi q}{n\sqrt{3}b}, \quad q = 1, 2, ..., 2n.
\]

The limit \(2n\) on \(q\) comes from the fact that \(k_{x,2n} = 4\pi/3b\), and \(k_{y,2n} = 4\pi/\sqrt{3}b\), and beyond these values one is outside of the first Brillouin zone of graphene.

5.24. Using (5.68) and (5.69), plot the dispersion curves for the first eight bonding and antibonding bands in a \((5,5)\), \((9,0)\), and \((10,0)\) carbon nanotube. Let the axial wavenumber vary from \(k = 0\) to \(k = \pi/a_{ac}\) for the armchair tube, and from \(k = 0\) to \(k = \pi/a_{zz}\) for the zigzag tube. Comment on whether each tube is metallic or semiconducting, and identify the band (i.e., the \(q\) value) that is most important. If the tube is semiconducting, determine the approximate band gap.

**Solution:** For the armchair tube \((5,5)\),

\[
E_{ac}(k_y) = \pm \gamma_0 \sqrt{1 + 4 \cos \left(\frac{\pi q}{n}\right) \cos \left(\frac{k_y a}{2}\right) + 4 \cos^2 \left(\frac{k_y a}{2}\right)}
\]

\[
= \pm \gamma_0 \sqrt{1 + 4 \cos \left(\frac{\pi q}{5}\right) \cos \left(\frac{k_y a}{2}\right) + 4 \cos^2 \left(\frac{k_y a}{2}\right)}
\]

\(-\pi < k_y a_{ac} < \pi, \quad q = 1, 2, ..., 2n, \text{ and so}\)

30
(vertical scale is $E/\gamma_0$). The $q = 5$ band (note that $n = 5!$) is the most important, since these bands cross in the first Brillouin zone (and hence, there is no band gap). The crossing point is $2/3$ of the way to the zone boundary, and so $k_F = 2\pi/3a$, such that the Fermi wavelength is $\lambda_F = 3a = 0.74$ nm.

For zigzag tubes,

$$E_{zz}(k_x) = \pm \gamma_0 \left[ 1 + 4 \cos \left( \frac{\sqrt{3}k_x a}{2} \right) \cos \left( \frac{\pi q}{n} \right) + 4 \cos^2 \left( \frac{\pi q}{n} \right) \right],$$

$-\pi < k_ya_{zz} < \pi$, $q = 1, 2, ..., 2n$. For the (9,0) tube,

where the $q = 6$ bands cross at $k = 0$, and, hence, this tube is metallic. For the (10,0) tube,
no bands cross, hence, the (10, 0) tube is a semiconductor. The \( q = 7 \) bands come the closest to each other (at \( k = 0 \)), and so the band gaps is \( 2E(k = 0) \) for \( q = 7 \), which is approximately 0.88 eV using \( \gamma_0 = 2.5 \) eV. It can be shown (See the book by Saito, Dresselhaus, and Dresselhaus, Reference [9] in Chapter 5) that

\[
E_g = \frac{2\gamma_0 a}{\sqrt{32r}},
\]

which for the (10, 0) tube (\( r = 0.391 \) nm) leads to 0.90 eV.

6 Problems Chapter 6: Tunnel Junctions and Applications of Tunneling

6.1. Plot the tunneling probability versus electron energy for an electron impinging on a rectangular potential barrier (Fig. 6.2, p. 185) of height \( 3 \) eV and width \( 2 \) nm. Assume that the energy of the incident electron ranges from \( 1 \) eV to \( 10 \) eV.

Solution:

\[
T = \frac{4E (E - V_0)}{V_0^2 \sin^2 (k_2a) + 4E (E - V_0)}, \quad k_2^2 = \frac{2m_e (E - V_0)}{h^2}
\]

\[
T = \frac{4E|q_e| (E|q_e| - 3|q_e|)}{3^2 |q_e|^2 \sin^2 \left( \frac{2m_e (E|q_e| - 3|q_e|)}{h^2} \right) (2 \times 10^{-9})} + 4E|q_e| (E|q_e| - 3|q_e|)
\]