Problem 1: Various

(a) What is a Shottky barrier between a metal and a semiconductor ?

Solution:

From Wikipedia: "A Schottky barrier, named after Walter H. Schottky, is a potential energy barrier for electrons formed at a metal-semiconductor junction. Schottky barriers have rectifying characteristics, suitable for use as a diode. One of the primary characteristics of a Schottky barrier is the Schottky barrier height, denoted by Φ_B. The value of Φ_B depends on the combination of metal and semiconductor.

Not all metal-semiconductor junctions form a rectifying Schottky barrier; a metal-semiconductor junction that conducts current in both directions without rectification, perhaps due to its Schottky barrier being too low, is called an ohmic contact."

(b) Derive the classical Drude formula for the electron conductivity σ based on Newton's second law:

$$\sigma = \frac{e^2 n\tau}{m}\,, \tag{1}$$

where τ is the typical scattering time between collisions, n is the electron density, e is (minus) the electron charge, and m is the electron mass. You should also state what the basic assumptions in deriving the Drude formula are.

Solution

In-between the scattering events, Newton's 2. law states that the acceleration of the electron at position $\mathbf{r}$ subject to an electric field $\mathbf{E}$ is

$$m\frac{d^2\mathbf{r}}{dt^2} = -e\mathbf{E}\,. \tag{2}$$

As a consequence, the velocity $\mathbf{v} = d\mathbf{r}/dt$ evolves in time as

$$\mathbf{v}(t) = \mathbf{v}(0) - t\frac{e}{m}\mathbf{E}\,, \tag{3}$$

where $\mathbf{v}(0)$ is the position at the initial time $t = 0$ just after the last scattering event. Our interest is in the average velocity obtained by averaging over many collisions

$$\mathbf{v}_{\text{avg}}(t) = \langle \mathbf{v}(t) \rangle \tag{4}$$

$$= \langle \mathbf{v}(0) \rangle - \langle t \rangle \frac{e}{m}\mathbf{E}\,. \tag{5}$$

Since the average initial velocity vanishes, $\langle \mathbf{v}(0) \rangle = 0$, and the typical scattering time is τ, $\langle t \rangle = \tau$, we find

$$\mathbf{v}_{\text{avg}} = -\tau \frac{e\mathbf{E}}{m} \tag{6}$$

so that the average current density $\mathbf{j} = -ne\mathbf{v}$ is

$$\mathbf{j} = \frac{e^2 n\tau}{m}\mathbf{E}\,, \tag{7}$$

which identifies the Drude conductivity via Ohm's law $\mathbf{j} = \sigma\mathbf{E}$ as

$$\sigma = \frac{e^2 n\tau}{m}\,. \tag{8}$$

(c) Consider a spin-degenerate ($g_s = 2$) free electron gas and compute the density of states as a function of energy ϵ, $D(\epsilon)$, when the system is three-dimensional with volume V.

Solution

We consider the system as a particle in a box with periodic boundary conditions. Along each of the three directions (i=1,2, or 3), the wave function is then of the form $\psi_i \sim \exp ik_i r_i$. The periodic boundary conditions dictate that $k_i = 2\pi n_i/L$, where n_i is an integral number. There is then 1 allowed $\mathbf{k}$-point in volume $(2\pi/L)^3$ in k-space. Since the spin degeneracy equals 2, the density of states in k-space is

$$D(k) = \frac{V}{4\pi^3} \tag{9}$$

and the number of k-states with a magnitude of k-vector smaller than k is

$$N(k) = D(k)V_3 \tag{10}$$

where the associated volume $V_3 = 4\pi k^3/3$ so that

$$N(k) = \frac{V}{3\pi^2}k^3\,. \tag{11}$$

The relation between the momentum $\mathbf{k}$ and energy ϵ is $\epsilon = \hbar^2 k^2/2m$ so that the number of states with an energy less than ϵ is

$$N(\epsilon) = \frac{V}{3\pi^2}\left(\frac{2m\epsilon}{\hbar^2}\right)^{3/2}\,. \tag{12}$$

The density of states is then

$$D(\epsilon) = \frac{dN(\epsilon)}{d\epsilon} = \frac{V}{2\pi^2}\left(\frac{2m}{\hbar^2}\right)^{3/2}\epsilon^{1/2}\,. \tag{13}$$

Problem 2: Transmission and Landauer-Büttiker conductance

Consider a spin-degenerate one-dimensional system attached to a left and a right reservoir. The Landauer-Büttiker conductance G is

$$G = \frac{2e^2}{h} T \,, \tag{14}$$

where e is (minus) the electron charge, h is Planck's constant, and $T = |t|^2$ is the transmission probability in terms of the transmission amplitude t.

(a) We now assume a particle with mass m and energy ϵ moves in a one-dimensional channel in the presence of a single scatterer with a potential

$$V(x) = V_0 \delta(x) \,, \tag{15}$$

where $\delta(x)$ is the Dirac-delta function $[\int_{-\infty}^{\infty} dx f(x)\delta(x-y) = f(y)]$ and V_0 is the strength of the scatterer with dimension $[V_0] = Jm$. We define a scattering matrix consisting of reflection r (r') and transmission amplitudes t (t') for electrons coming from the left (right) lead as

$$S = \begin{pmatrix} r & t' \\ t & r' \end{pmatrix} . \tag{16}$$

Show that the reflection amplitudes are

$$r = r' = \frac{V_0}{i\hbar v - V_0} \tag{17}$$

and the transmission amplitudes are

$$t = t' = \frac{i\hbar v}{i\hbar v - V_0} \,, \tag{18}$$

where the velocity $v = \sqrt{2E/m}$ is the same in both leads since the potential vanishes there.

Solution

The stationary Schrödinger equation is

$$\left[-\frac{\hbar^2}{2m} \frac{d^2}{dx^2} + V_0 \delta(x) \right] \psi(x) = \epsilon \psi(x) \,. \tag{19}$$

Let us first consider an incoming wave from the left. The wave function is

$$\psi(x) = \begin{cases} \frac{1}{\sqrt{k}} [\exp ikx + r \exp -ikx] & x < 0 \\ \frac{1}{\sqrt{k}} t \exp ikx & x > 0 \end{cases} \tag{20}$$

where $k = \sqrt{2m\epsilon}/\hbar$ is the wavevector which is related to the velocity via $v = \hbar k/m$. Continuity of the wave function gives

$$\psi(x = 0^+) = \psi(x = 0^-) \tag{21}$$

$$1 + r = t\,. \tag{22}$$

By integrating the Schrödinger equation (19) across the scatterer located at $x = 0$, we find

$$-\frac{\hbar^2}{2m}\left[\left(\frac{d\psi}{dx}\right)_{x=0^+} - \left(\frac{d\psi}{dx}\right)_{x=0^-}\right] + V_0\psi(x = 0) = 0 \tag{23}$$

$$-\frac{\hbar}{2}iv\,[t - (1 - r)] + V_0 t = 0 \tag{24}$$

From Eqs. (22) and (24) we find that

$$t = \frac{i\hbar v}{i\hbar v - V_0} \tag{25}$$

and

$$r = \frac{V_0}{i\hbar v - V_0} \tag{26}$$

Furthermore, since the system is mirror symmetric around $x = 0$, the reflection and transmission amplitudes associated with an incoming electron from the right are identical to the ones for an incoming electron from the left, $r = r'$ and $t = t'$.

(b) Imagine that we have two scatterers in series with scattering matrices S_1 and S_2, respectively. These two scatterers together define a total scattering matrix S_{12}.

Show that the reflection and transmission amplitudes of the total scattering matrix are

$$t_{12} = t_1[1 - r_2 r_1']^{-1} t_2 \tag{27}$$

$$r_{12} = r_1 + t_1 r_2 [1 - r_2 r_1']^{-1} t_1' \tag{28}$$

$$t_{12}' = t_2'[1 - r_1' r_2]^{-1} t_1' \tag{29}$$

$$r_{12}' = r_2' + t_2' r_1' [1 - r_1' r_2]^{-1} t_2 \tag{30}$$

in terms of the reflection and transmission amplitudes of the scattering matrices S_1 and S_2. It may be useful to know that $(1 - x)^{-1} = \sum_{i=0}^{\infty} x^i$.

Solution

Let us first consider the total transmission amplitude t_{12}. We sum over all possible ways to get through the scatterer from the left to the right:

$$t_{12} = t_1 t_2 + t_1 r_2 r_1' t_2 + t_1 r_2 r_1' r_2 r_1' t_2 + \ldots \tag{31}$$

$$t_{12} = t_1[1 - r_2 r_1']^{-1} t_2 \tag{32}$$

where we have used that $(1-x)^{-}1 = \sum_{i=0}^{\infty} x^i$. Similarly, we can find that the reflection amplitude for an imcoming electron from the left is

$$r_{12} = r_1 + t_1 r_2 t_1' + t_1 r_2 r_1' r_2 t_1' + \dots \tag{33}$$

$$r_{12} = r_1 + t_1 r_2 [1 - r_2 r_1']^{-1} t_1' \tag{34}$$

In the same way, we can find the reflection and transmission amplitudes associated with an incoming electron from the right (r_{12}' and t_{12}') by interchanging $r_1 \leftrightarrow r_2'$, $r_2 \leftrightarrow r_1'$, $t_1 \leftrightarrow t_2'$, and $t_2 \leftrightarrow t_1'$ with the result:

$$t_{12}' = t_2'[1 - r_1' r_2]^{-1} t_1' \tag{35}$$

$$r_{12}' = r_2' + t_2' r_1' [1 - r_1' r_2]^{-1} t_2 \tag{36}$$

(c) We now consider two identical scatterers in the one-dimensional channel located at $x = -a/2$ and $x = a/2$ with a total potential

$$V(x) = V_0 \delta(x + a/2) + V_0 \delta(x - a/2)\,. \tag{37}$$

As a scattering problem, we can now view the system as consisting of three scattering matrices in series where the leftmost and rightmost scattering matrices are identical to the one in problem a), $S_1 = S_3 = S$, and in the middle of the system ($-a/2 < x < a/2$), there is no reflection, but the transmission amplitude acquires a phase ka so that its scattering matrix is

$$S_2 = \begin{pmatrix} 0 & \exp ika \\ \exp ika & 0 \end{pmatrix} . \tag{38}$$

What is the total transmission *amplitude* for the whole system (consisting of scattering matrices S_1, S_2, and S_3) ? Show that the total transmission *probability* is

$$T_{123} = \frac{T^2}{1 - 2R\cos\theta + R^2} \tag{39}$$

where $\theta = 2\,[ka + \arctan \hbar v / V_0]$.

Solution

Let us first concatenate the scattering matrices S_1 and S_2. Since $r_2 = r_2' = 0$, Eq. (27) gives

$$t_{12} = t \exp ika\,, \tag{40}$$

$$r_{12} = r\,, \tag{41}$$

$$t'_{12} = t \exp ika\,, \tag{42}$$

$$r'_{12} = r \exp 2ika\,, \tag{43}$$

where the transmission t and reflection amplitudes r are defined in Eqs.(18) and (17), respectively.

Next, we concatenate the combined scattering matrix S_{12} with scattering matrix S_3 to find the total transmission amplitude t_{123} using Eq. (27):

$$t_{123} = t_{12}[1 - r_3 r'_{12}]^{-1} t_3 \tag{44}$$

$$t_{123} = t \exp ika[1 - rr \exp 2ika]^{-1} t \tag{45}$$

Making use of $r = \sqrt{R} \exp i\theta$ with $\theta = \arctan \hbar v/V_0$, we find the transmission probability

$$T_{123} = |t_{123}|^2 \tag{46}$$

$$T_{123} = \frac{|t \exp ika|^4}{[1 - R \exp{(2ika + 2i\theta)}][1 - R \exp{(-2ika - 2i\theta)}]} \tag{47}$$

$$T_{123} = \frac{T^2}{1 - 2R\cos\theta + R^2}\,. \tag{48}$$

(d) Consider that the transmission probability T for each scatterer is very small $T \ll 1$. What is the maximum transmission probability T_{123} and the associated Landauer-Büttiker conductance G for an arbitrary energy ϵ ? Comment on the physical interpretation of this result.

Solution

The maximum transmission probability

$$T_{123} = \frac{T^2}{1 - 2R\cos\theta + R^2} \tag{49}$$

is achieved when the denominator attains its minimum which is when $\theta = 0$. In this case, we have

$$T_{123} = \frac{T^2}{1 - 2R + R^2} \tag{50}$$

$$T_{123} = \frac{T^2}{(1 - R)^2} \tag{51}$$

$$T_{123} = 1 \tag{52}$$

Despite the fact that the transparancy of each scatterer is low, the total transmission probability $T_{123} = 1$ with an associated Landauer-Büttiker conductance that equals the conductance quantum $G = 2e^2/h$.

This is resonant tunneling and occors when the energy of the particle equals the resonant state between the scatterers. For instance, in the limit of an infinite strength of the scatterers $V_0 \to \infty$, the condition $\theta = 0$ implies that

$$ka = n\pi \tag{53}$$

so that the wave function is a standing wave between the scatterers. When the energy of the particle $\epsilon = \hbar^2 k^2/2m$ is in resonance with one of the bound states within the scatterers

$$\epsilon_n = \frac{\hbar^2}{2m}\frac{n^2\pi^2}{a^2}\,, \tag{54}$$

the transmission probability becomes equal to one.

Problem 3: Single-electron tunneling

Consider a junction that has a capacitance C and a large resistance R due to weak tunneling. Assume there is a charge Q to the left of the junction and a charge $-Q$ to the right of the junction. This charge may depend on time.

(a) Demonstrate that an energy $E_C = Q^2/2C$ is required to charge the capacitor from a zero charge to a charge Q.

Solution

For a capacitor, the charge Q is related to the voltage difference $V(Q)$ across the junction as $Q = CV(Q)$. The work to move one infinitesimal charge dq across the junction is $dqV(Q)$.

The energy cost associated with charging the capacitor from a zero charge to a charge Q is therefore

$$E_c = \int_0^Q dqV(q) = \int_0^Q dq\frac{q}{C} = \frac{Q^2}{2C}\,. \tag{55}$$

(b) At what thermal energies with respect to E_C do we expect single-electron tunneling effects to become important and why ?

Solution

At high temperatures $k_BT \gg E_c$, the effect of one extra electron on the capacitor is negligible as compared to the typical thermal energy fluctuations. The effect of the tunneling of a single electron can then not be seen.

When the temperature is low, $k_BT \ll E_C$, the energy change caused by tunneling of a single electron dominates. If this energy cannot be supplied by other parts of the circuit, there is no flow of electrons across the junction.

(c) Assume the junction (with capacitance C and tunnel resistance R) is an open circuit. Demonstrate that the typical decay time of the charge Q is $\tau = RC$.

Solution

The system is an open circuit. We define the potential so that it vanishes to the left of the junction and equals V to the right of the junction. The rate of change of the charge to the left of the junction is then

$$\frac{dQ}{dt} = -V(t)/R = -\frac{Q(t)}{RC} \tag{56}$$

so that the typical time constant is $\tau = RC$ and the evolution of the charge as a function of time is

$$Q(t) = Q(0)\exp -t/\tau\,, \tag{57}$$

where $Q(0)$ is the charge at $t = 0$.

(d) Find a condition using the tunnel conductance $G = 1/R$ when quantum flucutations can be avoided so that single-electron tunneling effects can be clearly seen.

Solution

The classical charging energy associated with the tunneling of one electron is $E_c = e^2/2C$. From Heisenberg's uncertainty relation, we have

$$\Delta\epsilon\Delta t \geq \hbar/2\,, \tag{58}$$

where $\Delta\epsilon$ is the energy uncertainty and Δt is the lifetime uncertainty. Since we know that the decay time is $\tau = RC$, we find that

$$\Delta\epsilon \geq \frac{\hbar}{2\tau}\,. \tag{59}$$

In order to clearly see single-electron tunneling effects these energy fluctuations must be smaller than the typical charging energy associated with a single electron, $\Delta\epsilon \ll E_C$.

This implies that

$$\frac{\hbar}{2\tau} \ll E_c \,. \tag{60}$$

Using $\tau = RC$ and $E_C = e^2/2C$ for a single-electron, we also find

$$G \ll \frac{2e^2}{h} \,. \tag{61}$$

In other words, the tunneling resistance must be large.