Departments of ECE and MSE, Cornell University

ECE 5390/MSE 5472: Quantum Transport in Electron Devices and Novel Materials
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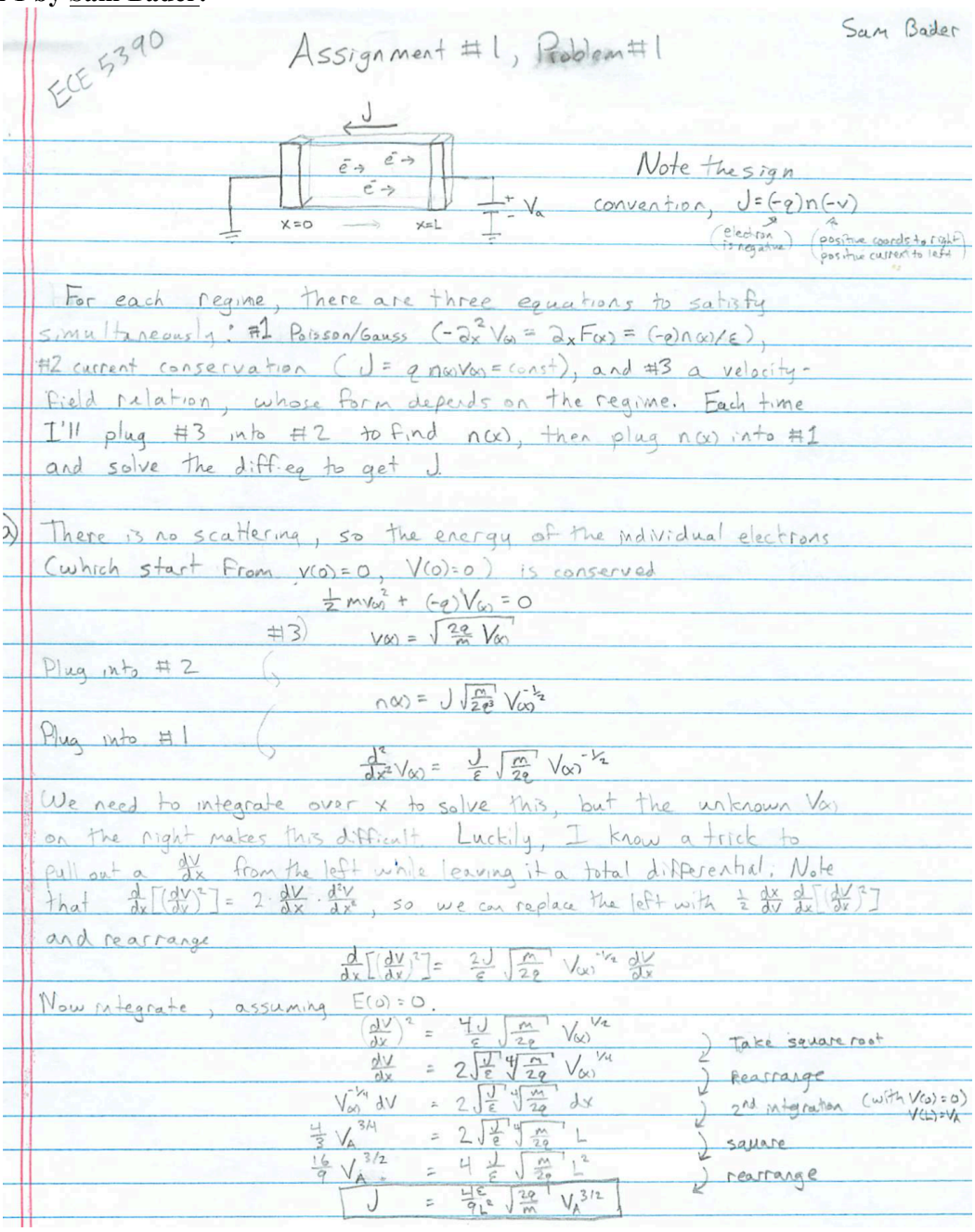
Assignment 1: Solutions

Problem 1.1) Ballistic vs. diffusive space-charge transport

Solution 1 by Sam Bader:



b) The scattering leads to a mobility μ such that

#3) $v(x) = -\mu F(x)$

Plug into #2 ↘

$$n(x) = -J/q\mu F(x)$$

Plug into #1 ↘

$$\frac{d}{dx}F(x) = J/\mu\varepsilon_s F(x)$$ ↘ rearrange

$$\mu\varepsilon_s F(x)\,dF = J\,dx$$ ↘ integrate with $F(0) = 0$

$$\tfrac{1}{2}\mu\varepsilon_s F(x)^2 = Jx$$ ↘ take square root + rearrange *

$$-F(x) = \sqrt{2Jx/\mu\varepsilon_s}\;x^{1/2}$$ ↘ 2nd integration with $V(0)=0$, $V(L)=a$

$$V_A = \tfrac{2}{3}\sqrt{2J/\mu\varepsilon_s}\;L^{3/2}$$ ↘ square

$$V_A^2 = \frac{8L^3}{9\mu\varepsilon_s}J$$ ↘ rearrang.

$$\boxed{J = \frac{9\mu\varepsilon_s}{8L^3}V_A^2}$$

* Note that we needed the negative root here because $F(x)$ should point left

c) If the velocity is saturated at $v = v_{sat}$, then, plugging into #2, the charge is constant at $n = J/qv_{sat}$, and, plugging into #1,

$$\frac{d}{dx}F(x) = -J/\varepsilon v_{sat}$$

$$F(x) = -(J/\varepsilon v_{sat})x$$

$$V_A = -(J/2\varepsilon v_{sat})L^2$$

$$\boxed{J = -\frac{2\varepsilon v_{sat}}{L^2}V_A}$$

d) None are Ohm's law because all have the wrong length dependance, and (a) & (b) have the wrong voltage dependence. The assumption underlying all three examples above differ from the Ohmic situation in that the region between the plates does not supply its own free carriers. So, in our examples, generating a current requires injecting charge into the middle region, which then reshapes the electric field according to Poisson's law. In contrast, an Ohmic material has free electrons with fixed nuclei, so there can be a flow of charge without having a net charge. So an ohmic material can still have $\partial F = 0$, ie a constant E-field, charge density, and electron velocity, leading to a simple current of $J = qnv = q\,n\,\mu E = qn\mu V/L$, and n is determined by the material, not by the voltage. Also none of these have an $\hbar$, because we treated the electrons as classical charged objects, and never involved any quantum mechanics.

Problem 1.2) Quantum Mechanics Recap

Solution by Rahul Sharma

Problem 1.2) Quantum Mechanics Recap

(a) In state n, the wavelength of an electron must satisfy $n\lambda_n = 2\pi r_n$ to close on itself for constructive interference for steady state.

$$\begin{aligned} p_n &= \frac{h}{\lambda_n} \\ L_n &= r_n \times p_n = \frac{n\lambda_n}{2\pi}\frac{h}{\lambda_n} = \frac{nh}{2\pi} \end{aligned}$$

$$\boxed{\therefore L_n = n\hbar}$$

Quantum case : $L_1 = \hbar = 1.05 \times 10^{-34} m^2 kg/s$
Classical case: $L = mvr = 1 m^2 kg/s$
Classical case is 10^{34} times larger !

(b) Balancing the force, we get :

$$\begin{aligned} ev_n B_n &= mv_n^2/r_n \\ \Longrightarrow B_n &= mv_n/er_n \\ B_n \cdot A &= \frac{mv_n}{er_n}\pi r_n^2 = \frac{\pi m v_n r_n}{e} = \frac{\pi L_n}{e} \\ \because L_n &= n\hbar \end{aligned}$$

$$\boxed{B_n \cdot A = \frac{\pi n\hbar}{e} = \frac{nh}{2e} = n\Phi_0}$$

(c) The state

$$\begin{aligned} \psi(x) &= a[\psi_1(x) + \psi_{-1}(x)] \\ &= \frac{a}{\sqrt{L}}\left[e^{i\frac{2\pi}{L}x} + e^{-i\frac{2\pi}{L}x}\right] \\ &= \frac{a}{\sqrt{L}} 2cos\left(\frac{2\pi}{L}x\right) \end{aligned}$$

Normalization requires

$$\begin{aligned} \int \psi(x)\psi^*(x) &= 1 \\ \Longrightarrow \frac{a^2}{L} 4 \int cos^2\left(\frac{2\pi}{L}x\right) &= 1 \\ \Longrightarrow \frac{a^2}{L} 4 \frac{L}{2} &= 1 \\ a &= \frac{1}{\sqrt{2}} \end{aligned}$$

If we apply momentum operator on $\psi(x)$, we get

$$\hat{P}\psi(x) = -i\hbar \frac{d}{dx}\frac{a}{\sqrt{L}} 2cos\left(\frac{2\pi}{L}x\right) = -i\hbar \frac{4\pi a}{L^{3/2}} sin\left(\frac{2\pi}{L}x\right) \neq const.\psi(x)$$

Hence $\psi(x)$ is not an eigenstate of momentum operator ! Therefore it does not have a definite momentum.

(d)

$$\hat{j}\psi_1(x) = \frac{-i\hbar}{2m}\left(e^{-i\frac{2\pi}{L}x}\frac{d}{dx}e^{i\frac{2\pi}{L}x} - e^{i\frac{2\pi}{L}x}\frac{d}{dx}e^{-i\frac{2\pi}{L}x}\right) = \frac{\hbar}{2m}\left(\frac{2\pi}{L} + \frac{2\pi}{L}\right)$$

$$\boxed{\therefore j_1 = \frac{h}{mL}}$$

$$\hat{j}\psi_{-1}(x) = \frac{-i\hbar}{2m}\left(e^{i\frac{2\pi}{L}x}\frac{d}{dx}e^{-i\frac{2\pi}{L}x} - e^{-i\frac{2\pi}{L}x}\frac{d}{dx}e^{i\frac{2\pi}{L}x}\right) = -\frac{\hbar}{2m}\left(\frac{2\pi}{L}+\frac{2\pi}{L}\right)$$

$$\boxed{\therefore j_{-1} = -\frac{h}{mL}}$$

$$\hat{j}\psi(x) = \hat{j}\frac{1}{\sqrt{2}}[\psi_1(x)+\psi_{-1}(x)] = \frac{1}{\sqrt{2}}[\hat{j}\psi_1(x)+\hat{j}\psi_{-1}(x)] \text{ (linear operator)}$$

$$= \tfrac{1}{\sqrt{2}}\ [j_1 + j_{-1}] = \frac{1}{\sqrt{2}}\left[\frac{h}{mL} - \frac{h}{mL}\right]$$

$$\boxed{\therefore j = 0}$$

The individual eigenstates ψ_1 and ψ_{-1} both carry current but equal and opposite in magnitude ! Hence their equal superposition leads to perfect cancellation of the current and we get 0 current in superposition state.

1.3) Tunneling and transmission

Solutions by Brian Schaefer:

1.3 Tunneling and transmission

Here you solve the problem of quantum mechanical tunneling of an electron through a barrier (see Figure 2). For an electron of mass m and kinetic energy E, write an expression for k. Also write an expression for k_b for a barrier height V_0. Explain when k_b is real and when it is imaginary.

$$E = \frac{\hbar^2 k^2}{2m} + V(x) \implies k(x) = \frac{\sqrt{2m[E - V(x)]}}{\hbar}$$

$$\boxed{k = \frac{\sqrt{2mE}}{\hbar} \qquad k_b = \frac{\sqrt{2m(E - V_0)}}{\hbar}}$$

k_b is imaginary if $\boxed{E < V_0}$, and real otherwise.

(a) There are 4 unknowns: the coefficients r, b, c, and t. Use boundary conditions that the wavefunction and its derivative are continuous at $x = +a/2$ and at $x = ?a/2$ to get 4 equations. Solving these 4 equations will yield the 4 unknown coefficients, solving the problem completely.

The four boundary conditions are:

$$e^{-ika/2} + re^{ika/2} = be^{-ik_b a/2} + ce^{ik_b a/2} \tag{1}$$

$$ike^{-ika/2} - ikre^{ika/2} = ik_b be^{-ik_b a/2} - ik_b ce^{ik_b a/2} \tag{2}$$

$$be^{ik_b a/2} + ce^{-ik_b a/2} = te^{ika/2} \tag{3}$$

$$ik_b be^{ik_b a/2} - ik_b ce^{-ik_b a/2} = ikte^{ika/2} \tag{4}$$

$ik(1) + (2) \implies$

$$2ike^{-ika/2} = i(k + k_b)be^{-ik_b a/2} + i(k - k_b)ce^{ik_b a/2} \tag{5}$$

$i(k - k_b)e^{ik_b a}(3) \implies$

$$i(k - k_b)be^{3ik_b a/2} + i(k - k_b)e^{ik_b a/2} = i(k - k_b)te^{3ika/2}$$

$(5) - i(k - k_b)e^{ik_b a}(3) \implies$

$$i(k + k_b)be^{-ik_b a/2} - i(k - k_b)be^{3ik_b a/2} = 2ike^{-ika/2} - i(k - k_b)te^{3ika/2} \tag{6}$$

$ik_b(3) + (4) \implies$

$$2ik_b be^{ik_b a/2} = i(k + k_b)te^{ika/2}$$

$$b = \frac{k + k_b}{2k_b} te^{i(k - k_b)a/2}$$

$ik_b(3) - (4) \implies$

$$2ik_b ce^{-ik_b a/2} = i(k_b - k)te^{ika/2}$$

$$c = \frac{k_b - k}{2k_b} te^{i(k + k_b)a/2}$$

Plugging b and c into (5),

$$2ike^{-ika/2} = i\frac{(k+k_b)^2}{2k_b}te^{ika/2}e^{-ik_ba} - i\frac{(k-k_b)^2}{2k_b}te^{ika/2}e^{ik_ba}$$

$$4kk_be^{-ika} = t\left[(k+k_b)^2e^{-ik_ba} - (k-k_b)^2e^{ik_ba}\right]$$

$$\boxed{t = \frac{4kk_be^{-ika}}{(k+k_b)^2e^{-ik_ba} - (k-k_b)^2e^{ik_ba}}}$$

The other three coefficients are algebraically tedious to find and not particularly illuminating.

(b) Since we are interested in the tunneling probability, explain why this probability is $T(E) = |t|^2$. Show then that it is given by the expression

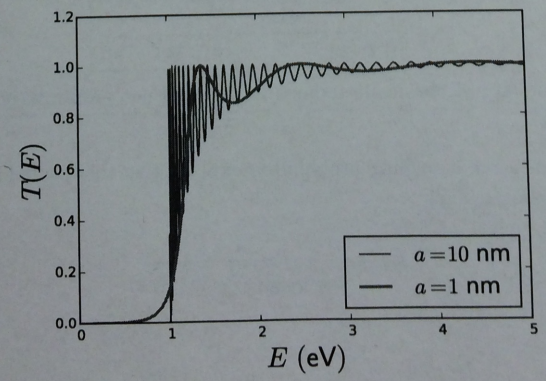
$$T(E) = \frac{1}{1 + \frac{V_0^2}{4E(E-V_0)}\sin^2(k_ba)}.$$

$$|t|^2 = tt^* = \frac{4kk_b e^{-ika}}{(k+k_b)^2 e^{-ik_b a} - (k-k_b)^2 e^{ik_b a}} \frac{4kk_b e^{ika}}{(k+k_b)^2 e^{ik_b a} - (k-k_b)^2 e^{-ik_b a}}$$
$$= \frac{16k^2 k_b^2}{(k-k_b)^4 + (k+k_b)^4 - (k+k_b)^2(k-k_b)^2(e^{-2ik_b a} + e^{2ik_b a})}$$

Using $2i\sin(x) = e^{ix} - e^{-ix} \implies -4\sin^2(x) = e^{2ix} + e^{-2ix} - 2$,

$$|t|^2 = \frac{16k^2 k_b^2}{2k^4 + 2k_b^4 + 12k^2 k_b^2 - (k^4 - 2k^2 k_b^2 + k_b^4)[2 - 4\sin^2(k_b a)]}$$
$$= \frac{8k^2 k_b^2}{k^4 + k_b^4 + 6k^2 k_b^2 - k^4 + 2k^2 k_b^2 - k_b^4 + 2(k^4 - 2k^2 k_b^2 + k_b^4)\sin^2(k_b a)}$$
$$= \frac{4k^2 k_b^2}{4k^2 k_b^2 + (k^4 - 2k^2 k_b^2 + k_b^4)\sin^2(k_b a)}$$
$$= \frac{1}{1 + \frac{(k^2 - k_b^2)^2}{4k^2 k_b^2}\sin^2(k_b a)}$$
$$= \frac{1}{1 + \frac{[E-(E-V_0)]^2}{4E(E-V_0)}\sin^2(k_b a)}$$
$$\boxed{= \frac{1}{1 + \frac{V_0^2}{4E(E-V_0)}\sin^2(k_b a)}}$$

(c) Note that when the kinetic energy of the electron is lower than the barrier, k_b is imaginary, and $\sin(iy) = i\sinh(y)$. Make a plot of the tunneling probability as a function of the electron energy E for a fixed barrier height $V_0 = 1$ eV. Use barrier thicknesses of $a = 10$ nm and $a = 1$ nm. Compare with my calculation shown in Figure 2. Note how sensitive tunneling is to thickness, and the resonances when $E > V_0$. These values are routinely encountered in semiconductor devices and nanostructures.

Explicitly writing $k_b = i\kappa$, where $\kappa = \sqrt{2m(V_0 - E)}/\hbar$ (real),

$$T(E) = \frac{1}{1 - \frac{V_0^2}{4E(E-V_0)}\sinh^2(\kappa a)}$$