ECE 5390 / MSE 5472, Fall Semester 2017

Quantum Transport in Electron Devices and Novel Materials

Debdeep Jena (djena@cornell.edu), Depts. Of ECE and MSE, Cornell University

Assignment 2, Solutions

Problem 2.1: The Harmonic Oscillator: Classical vs. Quantum

Problem 2.1) The Harmonic Oscillator: Classical vs. Quantum

In class we discussed that classically a mass oscillating in a harmonic oscillator potential is more likely to be found at the extremities of the oscillation when it has the highest potential energy and lowest kinetic energy. You also know the quantum wavefunction $\psi_n(x)$ of the quantum harmonic oscillator. Find the classical probability density $Pr_{cl}(x)$ of finding the mass classically between $(x, x + dx)$ and make a sketch. For the same oscillator and mass, make a plot of the quantum probability densities $Pr_{quantum}(x) = |\psi_n(x)|^2$ for a few n. Show that there is a correspondence between the quantum and classical results for large quantum numbers n, and significant deviation for small n.

Solution: [By Sayak Ghosh, 2017]

2.1) For classical harmonic oscillator, energy

$$E = \frac{p^2}{2m} + \frac{1}{2}m\omega^2 x^2$$

$$= \frac{1}{2}m\dot{x}^2 + \frac{1}{2}m\omega^2 x^2 \quad \text{is constant.} \quad \rightarrow (1)$$

Time period $= 2\pi/\omega$

If $(2\pi/\omega)$ time, the particle moves through every x twice.

So, probability of finding mass between x & $x+dx$,

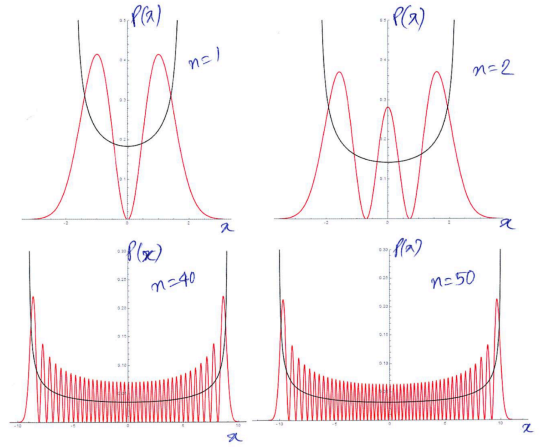
$$Pr_{cl}(x)\,dx = \frac{2\,dx/\dot{x}}{2\pi/\omega} \Rightarrow Pr_{cl}(x) = \frac{\omega}{\pi\dot{x}}$$

from (1), $\dot{x} = \sqrt{\left(E - \frac{1}{2}m\omega^2 x^2\right)\frac{2}{m}}$

$$\therefore \boxed{Pr_{cl}(x) = \frac{1}{\pi\sqrt{\frac{2E}{m\omega^2} - x^2}} = \frac{1}{\pi\sqrt{x_0^2 - x^2}}} \quad \left(x_0^2 = \frac{2E}{m\omega^2} \text{ is the turning point}\right)$$

From the plots, we can clearly see that $Pr_{cl}(x)$ is close to $Pr_{quantum}(x)$ for large n, and is quite different for small n. (Please find plots at end).

2.1) Classical and Quantum Oscillator.



Red → $Pr_{quantum}(x)$, Black → $Pr_{cl}(x)$

Clearly, the curves look similar for large n, and much different for small n.

We use $E_n = \left(n+\frac{1}{2}\right)\hbar\omega$ to compare Pr_{cl} to $Pr_{quantum}$. Putting this E,

$$Pr_{cl}(x) = \frac{1}{\pi\sqrt{(2n+1)\frac{\hbar}{m\omega} - x^2}}$$

for plotting easily, we use $\frac{\hbar}{m\omega} = 1$.

Problem 2.2: Second Quantization Methods

Problem 2.2) Second Quantization Methods

To handle interactions between many particles, we introduced the occupation-number (or Fock-space) formalism of quantum mechanics through the creation and annihilation operators that obeyed the relations $[b_i, b_j^\dagger] = b_i b_j^\dagger - b_j^\dagger b_i = \delta_{ij}$ for Bosons, and $\{c_i, c_j^\dagger\} = c_i c j^\dagger + c_j^\dagger c_i = \delta_{ij}$ for Fermions. The creation and annihilation operators follow the ladder operations $b^\dagger|n\rangle = \sqrt{n+1}|n+1\rangle$ and $b|n\rangle = \sqrt{n}|n-1\rangle$ for bosons, and corresponding relations for Fermions. The Pauli-exclusion principle is built into this formalism from the get-go because the occupation number of an orbital for Fermions can be only 0, or 1, the only possible eigenvalues of the occupation number operator $\hat{N} = c^\dagger c$.

For Bosons, we could create a Fock-state $|\Psi\rangle = |n_1, n_2, ..., n_k, ...\rangle$ by repeated application of the creation operator on the Vacuum state: $|\Psi\rangle = |n_1, n_2, ..., n_k, ...\rangle = \frac{(b_k^\dagger)^{n_k}}{\sqrt{n_k!}} ... \frac{(b_2^\dagger)^{n_2}}{\sqrt{n_2!}} \frac{(b_1^\dagger)^{n_1}}{\sqrt{n_1!}}|0\rangle$. Since the Bosonic creation and annihilation operators of different orbitals *commute*, we do not have to worry about the *order* in which the creation operators act on the vacuum state. The vacuum state $|0\rangle = |0, 0, 0, ...\rangle$ has all orbitals unoccupied, and formally looks the same for Bosons and Fermions. Similarly, we could create a Fermionic Fock state by repeated application of the creation operators on $|0\rangle$, but since the creation operators of different orbitals *anti-commute*, we have to pay special attention to the ordering: $|\Psi\rangle = |n_1, n_2, ..., n_k, ...\rangle = (c_k^\dagger)^{n_k} ... (c_2^\dagger)^{n_2} (c_1^\dagger)^{n_1}|0\rangle$. Note that since $n_j = 0$ or 1 for Fermions, $\sqrt{n_j!} = 1$ for all, so we do not need to write out the factorials.

(a) Show that the fermion anti-commutator algebra directly implies $(\hat{c}_\lambda^\dagger)^2 = 0$. Argue why this is nothing but the Pauli exclusion principle for fermions, meaning $\hat{n}_\lambda = \hat{c}_\lambda^\dagger \hat{c}_\lambda$ acting on fermion eigenstates can only produce eigenvalues 0 or 1, unlike $0, 1, 2, ...$ for bosons.

Evaluate the following matrix elements (Note that $a = b$ and $a^\dagger = b^\dagger$ for bosons, and $a = c$ and $a^\dagger = c^\dagger$ for Fermions, a is simply a more general creation/annihilation operator symbol):

(b) $\langle 1, 1|a_1^\dagger a_2^\dagger a_1 a_2|1, 1\rangle$ for Bosons ($a = b$), and then Fermions ($a = c$), and compare the results with $\langle 1, 1|a_1^\dagger a_1 a_2^\dagger a_2|1, 1\rangle$.

(c) $\sum_{j=1}^{\infty}\langle ...0_{k+1}, 1_k, ..., 1_2, 0_1|a_j^\dagger a_j|0_1, 1_2, ..., 1_k, 0_{k+1}, ...\rangle$ for Fermions and then for Bosons.

The ground state of an electron (Fermion) system may be written as $|\Phi\rangle = |1_1, 1_2, ..., 1_N, 0_{N+1}, ...\rangle$, where N is the highest occupied orbital (its energy E_N is the Fermi energy). Work out the following matrix element sums for $|\Phi\rangle$:

(d) $\sum_{j,k,l,m}^{\infty}\langle\Phi|a_j^\dagger a_k^\dagger a_l a_m|\Phi\rangle = 0$.

(e) $\sum_{j=1}^{N}\sum_{k=1}^{N}\sum_{l=1}^{N}\sum_{m=1}^{N}\langle\Phi|e^{i(l-k)x}a_j^\dagger a_k^\dagger a_l a_m|\Phi\rangle = N^2 - \frac{\sin^2(\frac{Nx}{2})}{\sin^2(\frac{x}{2})} = G_N(x)$. Make a sketch of the function $\frac{G_N(x)}{N^2}$ as a function of x for various (large) values of N. This function is called the pair-correlation function.

Solution: [By Sam Bader, 2015]

a)

The fermionic algebra satisfies

$$c_i, c_j^\dagger = \delta_{ij}, \quad c_i, c_j = 0, \quad c_i^\dagger, c_j^\dagger = 0$$

If we examine the last of those for the case $i = j$, we have $c_i^\dagger c_i^\dagger + c_i^\dagger c_i^\dagger = 0$, ie $2c_i^\dagger c_i^\dagger = 0$, ie $(c_i^\dagger)^2 = 0$. Since $c_i^\dagger$ creates a particle in the i state, $(c_i^\dagger)^2$ would double-populate the i state. The fact that this product is zero means that a double-populated (or even further overpopulated) state is unreachable through these operators. That is to say, if all the physics is expressed in terms of fermionic creation and annihilation operators (and some validly-occupied ground state), then no state can ever be occupied by more than one such fermion: this is the Pauli principle.

b)

First, I'll demonstrate the number operator $a_i^\dagger a_i$ does what its name suggests regardless of the particle statistics.

For bosons, a state can be written $|\psi\rangle = \prod_j \frac{(b_j^\dagger)^{n_j}}{\sqrt{n_j}}|0\rangle$. Apply the number operator

$$b_i^\dagger b_i|\psi\rangle = b_i^\dagger b_i \prod_j \frac{(b_j^\dagger)^{n_j}}{\sqrt{n_j}}|0\rangle$$

. The b_i can commute freely past all but n_i the $b_i^\dagger$ operators in front of. It picks up a 1 from each of those n_i commutators.

$$b_i^\dagger b_i|\psi\rangle = n_i b_i^\dagger \prod_j \frac{(b_j^\dagger)^{n'_j}}{\sqrt{n_j}}|0\rangle$$

. where $n'_j = n_j - \delta_{ij}$. Then the $b_i^\dagger$ from the number operator commutes over to replace the missing $b_i^\dagger$ from the state.

$$b_i^\dagger b_i|\psi\rangle = n_i \prod_j \frac{(b_j^\dagger)^{n_j}}{\sqrt{n_j}}|0\rangle = n_i|\psi\rangle$$

For fermions, the state can be written $|\psi\rangle = \prod_j (c_j^\dagger)^{n_j}|0\rangle$. Apply the number operator

$$c_i^\dagger c_i|\psi\rangle = c_i^\dagger c_i \prod_j (c_j^\dagger)^{n_j}|0\rangle$$

The c_i moves past all the $j \neq i$ operators picking up some number m of minus signs I won't bother specifying because it won't matter, on its way to the possibly present $c_i^\dagger$. It only picks up a 1 from the anticommutator if there is an i particle present ($n_i = 1$), then continues on to annihilate the ground state. Then, if the result is still non-zero the $c_i^\dagger$ from the number operator commutes through to replace the possibly eliminated $c_i^\dagger$ from the state, picking up the same m minus signs. So

$$c_i^\dagger c_i|\psi\rangle = n_i \prod_j (c_j^\dagger)^{n_j}|0\rangle$$

Now, this problem is straghtforward. The matrix element $\langle 1,1|a_1^\dagger a_1 a_2^\dagger a_2|1,1\rangle$ is simply two number operators in sequence, and there's a particle in each state, so, regardless of the particle statistics, $\langle 1,1|a_1^\dagger a_1 a_2^\dagger a_2|1,1\rangle = 1$. The matrix element $\langle 1,1|a_1^\dagger a_2^\dagger a_1 a_2|1,1\rangle$ is the same but an a_1 and $a_2^\dagger$ have been switched. For bosons, these commute, so it doesn't matter. For fermions, these anticommute, so we pick up one sign.

In summary

$$\langle 1,1|b_1^\dagger b_2^\dagger b_1 b_2|1,1\rangle = 1$$

$$\langle 1,1|c_1^\dagger c_2^\dagger c_1 c_2|1,1\rangle = -1$$

$$\langle 1,1|b_1^\dagger b_1 b_2^\dagger b_2|1,1\rangle = 1$$

$$\langle 1,1|c_1^\dagger c_1 c_2^\dagger c_2|1,1\rangle = 1$$

c)

Given the demonstration of the number operator from (b), this is easy.

$$\sum_{j=1}^{\infty}\langle 0_1, 1_2 \ldots 1_k, 0_{k+1}, \ldots |a_j^\dagger a_j|0_1, 1_2 \ldots 1_k, 0_{k+1}, \ldots\rangle$$

$$= \sum_{j=1}^{\infty}\langle 0_1, 1_2 \ldots 1_k, 0_{k+1}, \ldots |n_j|0_1, 1_2 \ldots 1_k, 0_{k+1}, \ldots\rangle$$

where n_j is 1 for $1 < j \leq k$

$$= \sum_{j=1}^{\infty} n_j$$

$$= k - 1$$

d)

$$\sum_{jklm}^{\infty}\langle\Phi|a_j^\dagger a_k^\dagger a_l a_m|\Phi\rangle$$

Unless the destruction operators for l and m are countered by matching creation operators, $(a_l a_m|\Phi\rangle)$ and $(\langle\Phi|a_j^\dagger a_k^\dagger)$ are orthogonal. So we must have $j = m, k = l$ or $j = l, k = m$. We can break the non-zero contributions to this sum into those two options, being careful not to double count the

terms with $j = k = l = m$. (I'll pull out these terms to a separate sum.)

$$= \sum_{jk}^{\infty} \langle \Phi | \left[a_j^\dagger a_k^\dagger a_k a_j (1 - \delta_{jk}) + a_j^\dagger a_k^\dagger a_j a_k (1 - \delta_{jk}) \right] | \Phi \rangle + \sum_{j}^{\infty} \langle \Phi | a_j^\dagger a_j^\dagger a_j a_j | \Phi \rangle$$

The second sum vanishes because it contains two of the same creation operators in sequence, which we argued in (a) is zero.

$$= \sum_{jk}^{\infty} \langle \Phi | \left[a_j^\dagger a_k^\dagger a_k a_j (1 - \delta_{jk}) + a_j^\dagger a_k^\dagger a_j a_k (1 - \delta_{jk}) \right] | \Phi \rangle$$

Let's do some anticommutations on the left to produce number operators. This requires an even number of anticommutations on the first term, and odd on the second.

$$= \sum_{jk}^{\infty} \langle \Phi | \left[a_k^\dagger a_k a_j^\dagger a_j (1 - \delta_{jk}) - a_k^\dagger a_k a_j^\dagger a_j (1 - \delta_{jk}) \right] | \Phi \rangle$$

We see that these terms are the same but for their sign.

$$= 0$$

e)

$$\sum_{jklm}^{N} \langle \Phi | e^{i(l-k)x} a_j^\dagger a_k^\dagger a_l a_m | \Phi \rangle$$

We can make the exact same arguments and commutations as in (d) to reduce the problem to

$$= \sum_{jk}^{N} \langle \Phi | \left[a_k^\dagger a_k a_j^\dagger a_j (1 - \delta_{jk}) - e^{i(j-k)x} a_k^\dagger a_k a_j^\dagger a_j (1 - \delta_{jk}) \right] | \Phi \rangle$$

where the only difference from (d) is that a phase is now carried on the second term (this phase vanished from the first term becase that term came from $k = l$). Using the fact that $|\Phi\rangle$ is occupied up to N:

$$= \sum_{jk}^{N} (1 - \delta_{jk})(1 - e^{i(j-k)x})$$

And the $(1 - e^{i(j-k)x})$ factor vanishes for $j = k$ so we can drop the $(1 - \delta_{jk})$

$$= \sum_{jk}^{N} (1 - e^{i(j-k)x})$$

There are N^2 terms in this sum

$$= N^2 - \sum_{jk}^{N} e^{i(j-k)x}$$

$$= N^2 - \left(\sum_{k}^{N} e^{-ikx} \right) \left(\sum_{j}^{N} e^{ijx} \right)$$

$$= N^2 - \left(e^{-ix} \frac{1 - e^{-iNx}}{1 - e^{-ix}} \right) \left(e^{ix} \frac{1 - e^{iNx}}{1 - e^{ix}} \right)$$

We can pull out phases from each parenthesized term, which conveniently cancel each other

$$= N^2 - \left(\frac{e^{iNx/2} - e^{-iNx/2}}{e^{ix/2} - e^{-ix/2}} \right) \left(\frac{e^{-iNx/2} - e^{iNx/2}}{e^{-ix/2} - e^{ix/2}} \right)$$

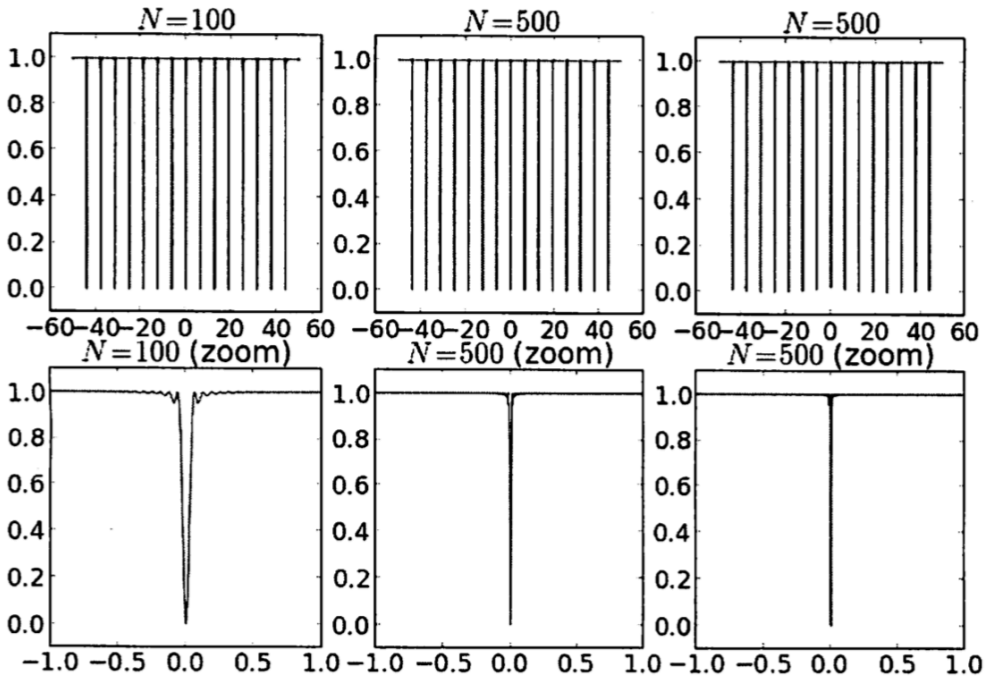
$$= N^2 - \left(\frac{2i \sin(Nx/2)}{2i \sin(x/2)} \right) \left(\frac{-2i \sin(Nx/2)}{-2i \sin(ix/2)} \right)$$

$$= N^2 - \frac{\sin^2(Nx/2)}{\sin^2(x/2)}$$

```
def plotGN(N,zoom=False):
    x=linspace(-50,50,100000)
    if zoom:
        x=linspace(-1,1,100000)
    plot(x,(N**2-sin(N*x/2)**2/sin(x/2)**2)/N**2)
    ylim(-.1,1.1)

figure(figsize=(11,2))
subplot(231)
plotGN(100)
title('$N=100$')

subplot(232)
plotGN(500)
```

```
title('$N=500$')

subplot(233)
plotGN(1000)
title('$N=500$')

subplot(234)
plotGN(100,zoom=True)
title('$N=100$ (zoom)')

subplot(235)
plotGN(500,zoom=True)
title('$N=500$ (zoom)')

subplot(236)
plotGN(1000,zoom=True)
title('$N=500$ (zoom)')
```

```
<matplotlib.text.Text at 0x7f1507f4e550>
```



The zoomed out images look the same, G_N is essentially 1 everywhere except in the vicinity of multiples of 2π where the second term has a near-divergence (cut off by N) which cancels the first term and brings the G_N to zero. If we zoom in on these spikes, we see that larger values of N make the spikes sharper. (One could see this analytically by applying L'Hopital's rule.)

The plots above are normalized by the particle number.

Problem 2.3: Bandstructure and Quasiparticles

Problem 2.3) Bandstructure and Quasiparticles

In class we discussed writing the single-particle tight-binding Hamiltonian for electrons on a linear chain of atoms with lattice constant a as $\hat{H}_{el} = \sum_n \left(E_0 c_n^\dagger c_n - t_0 c_{n+1}^\dagger c_n - t_0 c_{n-1}^\dagger c_n \right)$.

(a) Explain the meaning of this form of Hamiltonian, and the approximation made to write it in this form.

(b) Now Fourier-transform the on-site orbital indexed creation/annihilation operators $c_n^\dagger$ and c_n to the $|k\rangle$ orbital indexed creation/annihilation operators $c_k^\dagger$ and c_k, and show that the Hamiltonian is then diagonalized to the form $\hat{H}_{el} = \sum_k E(k) c_k^\dagger c_k$, where the bandstructure, or electron energy dispersion is given by $E(k) = E_0 - 2t_0 \cos(ka)$. This is a typical model of a one-orbital band.

Solve the following simple yet profound problem. In the Bardeen-Cooper-Schrieffer (BCS) theory of superconductivity, the annihilation and creation operators for a correlated pair of electrons of opposite spins (the Cooper-pair) are defined by $\hat{a}_{\mathbf{k}} = \hat{c}_{-\mathbf{k},\downarrow} \hat{c}_{\mathbf{k},\uparrow}$ and $\hat{a}_{\mathbf{k}}^\dagger = \hat{c}_{\mathbf{k},\uparrow}^\dagger \hat{c}_{-\mathbf{k},\downarrow}^\dagger$.

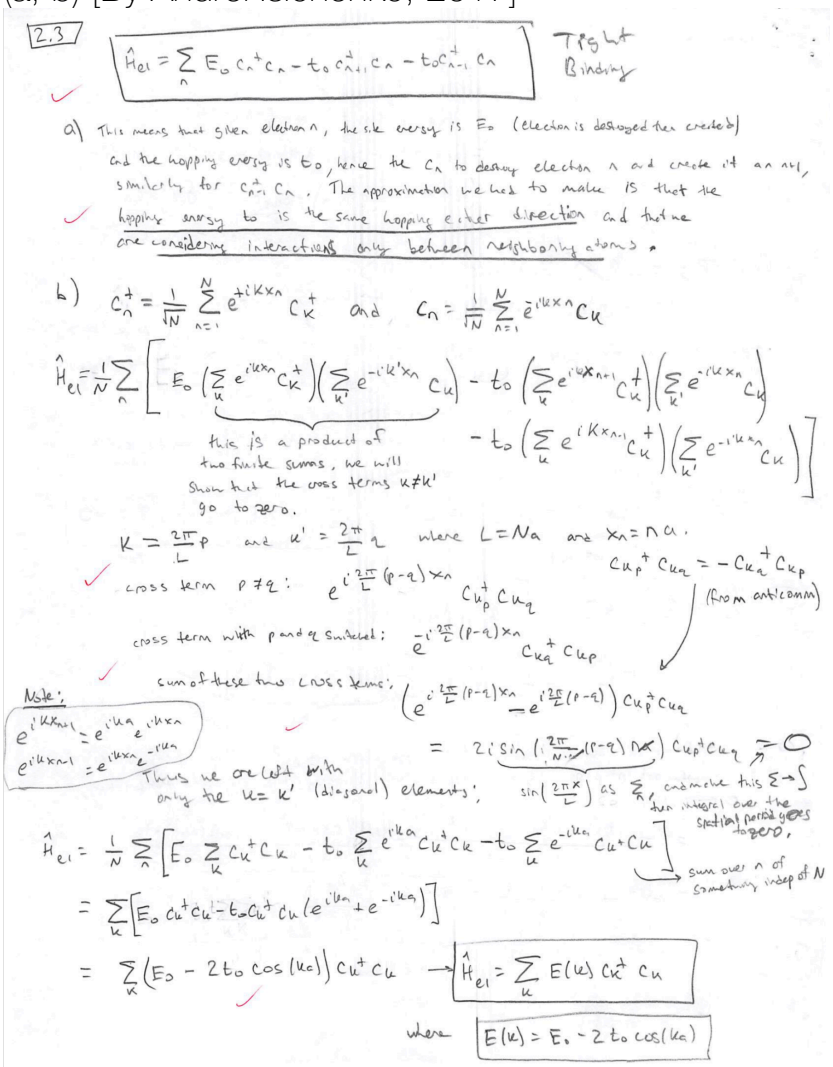
(c) Show that $[\hat{a}_{\mathbf{k}}, \hat{a}_{\mathbf{k}'}] = [\hat{a}_{\mathbf{k}}^\dagger, \hat{a}_{\mathbf{k}'}^\dagger] = 0$.
(d) Show that $[\hat{a}_{\mathbf{k}}, \hat{a}_{\mathbf{k}'}^\dagger] = \delta_{\mathbf{k},\mathbf{k}'}(1 - \hat{n}_{-\mathbf{k},\downarrow} - \hat{n}_{\mathbf{k},\uparrow})$.
(e) Show that $\{\hat{a}_{\mathbf{k}}, \hat{a}_{\mathbf{k}'}\} = 2\hat{a}_{\mathbf{k}}\hat{a}_{\mathbf{k}'}(1 - \delta_{\mathbf{k},\mathbf{k}'})$.

(f) Argue from the above algebra that Cooper pairs *seem* to follow boson algebra for 'hole' states, when $\hat{n}_{-\mathbf{k},\downarrow} = \hat{n}_{\mathbf{k},\uparrow} = 0$, *even though they are made of fermions!* But also argue why their creation/annihilation algebra is not *exactly* bosonic.

(g) Discuss how particles of different types (fermions & bosons) may be treated by the 2nd quantization techniques. Identify the importance of diagonalization of the many-particle Hamiltonians, and how this process predicts quasiparticles such as excitons, polarons, or polaritons - all of which have been experimentally observed.

Solution:

(a, b) [By Andrei Isichenko, 2017]



(c) [By Sam Bader, 2015]

$$[a_k, a_{k'}] = c_{-k,\downarrow}c_{k,\uparrow}c_{k',\uparrow}c_{-k',\downarrow} - c_{k',\uparrow}c_{-k',\downarrow}c_{-k,\downarrow}c_{k,\uparrow} = c_{-k,\downarrow}c_{k,\uparrow}c_{k',\uparrow}c_{-k',\downarrow} - c_{-k,\downarrow}c_{k,\uparrow}c_{k',\uparrow}c_{-k',\downarrow} = 0$$

where the middle equality proceeds because it takes an even number of anticommutations to reorder the second term.

Also, the exact same math goes through if we put a dagger on every operator:

$$[a_k^\dagger, a_{k'}^\dagger] = 0$$

(d)

$$\begin{aligned}
&[a_k, a_{k'}^\dagger] \\
&= c_{-k,\downarrow}c_{k,\uparrow}c_{k',\uparrow}^\dagger c_{-k',\downarrow}^\dagger - c_{k',\uparrow}^\dagger c_{-k',\downarrow}^\dagger c_{-k,\downarrow}c_{k,\uparrow} \\
&= c_{-k,\downarrow}c_{-k',\downarrow}^\dagger c_{k,\uparrow}c_{k',\uparrow}^\dagger - c_{k',\uparrow}^\dagger c_{-k',\downarrow}^\dagger c_{-k,\downarrow}c_{k,\uparrow} \\
&= (-c_{-k',\downarrow}^\dagger c_{-k,\downarrow} + \delta_{kk'})c_{k,\uparrow}c_{k',\uparrow}^\dagger - c_{k',\uparrow}^\dagger c_{-k',\downarrow}^\dagger c_{-k,\downarrow}c_{k,\uparrow} \\
&= (-c_{-k',\downarrow}^\dagger c_{-k,\downarrow} + \delta_{kk'})(-c_{k',\uparrow}^\dagger c_{k,\uparrow} + \delta_{kk'}) - c_{k',\uparrow}^\dagger c_{-k',\downarrow}^\dagger c_{-k,\downarrow}c_{k,\uparrow} \\
&= c_{-k',\downarrow}^\dagger c_{-k,\downarrow}c_{k',\uparrow}^\dagger c_{k,\uparrow} + (1 - c_{-k,\downarrow}^\dagger c_{-k,\downarrow} - c_{k',\uparrow}^\dagger c_{k,\uparrow})\delta_{kk'} - c_{k',\uparrow}^\dagger c_{-k',\downarrow}^\dagger c_{-k,\downarrow}c_{k,\uparrow} \\
&= c_{-k',\downarrow}^\dagger c_{-k,\downarrow}c_{k',\uparrow}^\dagger c_{k,\uparrow} + (1 - c_{-k,\downarrow}^\dagger c_{-k,\downarrow} - c_{k',\uparrow}^\dagger c_{k,\uparrow})\delta_{kk'} - c_{-k',\downarrow}^\dagger c_{-k,\downarrow}c_{k',\uparrow}^\dagger c_{k,\uparrow}
\end{aligned}$$

$$= (1 - c^\dagger_{-k,\downarrow} c_{-k,\downarrow} - c^\dagger_{k',\uparrow} c_{k,\uparrow})\delta_{kk'}$$
$$= (1 - n_{-k,\downarrow} - n_{k',\uparrow})\delta_{kk'}$$

(e)

$$\{a_k, a_{k'}\}$$
$$= c_{-k,\downarrow} c_{k,\uparrow} c_{-k',\downarrow} c_{k',\uparrow} + c_{-k',\downarrow} c_{k',\uparrow} c_{-k,\downarrow} c_{k,\uparrow}$$
$$= c_{-k,\downarrow} c_{k,\uparrow} c_{-k',\downarrow} c_{k',\uparrow} - c_{-k',\downarrow} c_{-k,\downarrow} c_{k',\uparrow} c_{k,\uparrow}$$
$$= c_{-k,\downarrow} c_{k,\uparrow} c_{-k',\downarrow} c_{k',\uparrow} - (-c_{-k,\downarrow} c_{-k',\downarrow} + \delta_{kk'}) c_{k',\uparrow} c_{k,\uparrow}$$

If $k = k'$, then we have a repeated fermionic operator ($c_{k,\uparrow} c_{k,\uparrow}$), so that term would be zero.

$$= c_{-k,\downarrow} c_{k,\uparrow} c_{-k',\downarrow} c_{k',\uparrow} + c_{-k,\downarrow} c_{-k',\downarrow} c_{k',\uparrow} c_{k,\uparrow}$$
$$= c_{-k,\downarrow} c_{k,\uparrow} c_{-k',\downarrow} c_{k',\uparrow} + c_{-k,\downarrow} c_{-k',\downarrow} (-c_{k,\uparrow} c_{k',\uparrow} + \delta_{kk'})$$

If $k = k'$, then we have a repeated fermionic operator ($c_{-k,\downarrow} c_{-k,\downarrow}$), so that term would be zero.

$$= c_{-k,\downarrow} c_{k,\uparrow} c_{-k',\downarrow} c_{k',\uparrow} - c_{-k,\downarrow} c_{-k',\downarrow} c_{k,\uparrow} c_{k',\uparrow}$$
$$= c_{-k,\downarrow} c_{k,\uparrow} c_{-k',\downarrow} c_{k',\uparrow} + c_{-k,\downarrow} c_{k,\uparrow} c_{-k',\downarrow} c_{k',\uparrow}$$
$$= 2a_k a_{k'}$$

Note $a_k a_{k'} = c_{-k,\downarrow} c_{k,\uparrow} c_{-k',\downarrow} c_{k',\uparrow} = -c_{-k,\downarrow} c_{-k',\downarrow} c_{k,\uparrow} c_{k',\uparrow}$, which is clearly zero if $k = k'$ due to the repeated fermionic operators. So the fact that this commutator is zero for $k = k'$ is already built into $a_k a_{k'}$. Thus it wouldn't change our answer at all to explictly include a factor which is one for $k \neq k'$, and zero for $k = k'$.

$$= 2a_k a_{k'}(1 - \delta_{kk'})$$

(f)

When restricted to hole states (for which a_k and n_k vanish), the above relations become

$$[a_k, a_{k'}] = [a^\dagger_k, a^\dagger_{k'}] = 0$$
$$[a_k, a^\dagger_{k'}] = \delta_{kk'}$$
$$\{a_k, a^\dagger_{k'}\} = 0$$

That is the algebra of bosonic operators. However, to truly be bosonic, these relations would need to hold on the full space of possible states.

(g)

It turns out that there are many electrons, phonons, and photons in any actual material, and, unfortunately, they interact. Because life is hard sometimes. Finding the energy spectrum of an actual material is thus a process of diagonalizing a many-body Hamiltonian. However, given simple enough models of the interactions, this diagonalization often leads approximately to combinations of true single-particle operators which behave compositely in simple ways. A fine example being the emergence of the Cooper pairs, which behave (sort of) like a single boson from the many-body interactions of electrons. Excitons (electron-hole combinations), polarons (electron - polar phonon combinations), and polaritons (photon - polar phonon combinations) are other examples of this procedure.

Problem 2.4: Quantum Transport by Tunneling, Transmission, and Thermionic Emission

Problem 2.4) Quantum Transport by Tunneling, Transmission, and Thermionic Emission

From the handouts, solve the following problems:

(a) Kroemer, Problem 5.5-1, page 161.

(b) Kroemer, Problem 6.4-1, page 181.

(c) Lundstrom, Problem 1.15, page 53.

Solution:

(a) [by Sayak, 2017]

◆ **PROBLEM TO SECTION 5.5**

#5•5-1: Transmission Properties of a Composite Barrier

Consider a composite barrier of the general type shown in **Fig. 5•5–2**, containing N discontinuities separating by $N + 1$ flat-potential sections.

The propagation matrix of such a structure has the form

$$\hat{P} = \hat{D}^{(1)} \cdot \hat{F}^{(1)} \cdot \hat{D}^{(2)} \cdot \ldots \cdot \hat{F}^{(N-1)} \cdot \hat{D}^{(N)}, \qquad (5•5–7)$$

where the $\hat{D}$'s are the propagation matrices associated with the discontinuities and the $\hat{F}$'s are associated with the flat-potential sections.

(a) Write a computer program that determines the current transmission probability T as a function of the incident energy $\mathcal{E}$, for a potential that contains an arbitrary number of discontinuities with arbitrary lengths L_n and arbitrary potential energies V_n.

(b) Execute the program for the following four-step potential

n:	0	1	2	3	4
L_n[nm]:	0	1	2	3	0
V_n[eV]:	0	+1	−2	0	−1

Calculate and plot T for this potential, in the incident energy range $0 \le \mathcal{E} \le 2$ eV, in steps no coarser than 0.1 eV. *Note:* The choice of the length L_N of the exit side of the potential is irrelevant, but specifying a zero length is a convenient way to signal the end of the composite barrier to the program, without having to specify the number of potential steps beforehand.

(c) Re-run the program in the energy range appropriate for bound states of the structure. Plot T vs. $\mathcal{E}$ in that range, and determine the energy of any bound states that might be present, to better than ±0.05 eV. Also, explore the existence of quasi-bound states showing up as resonances in T, with $T < \infty$ in the energy range $0 > \mathcal{E} > V_4$.

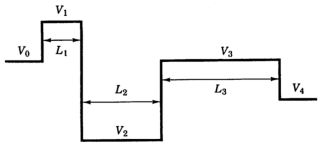
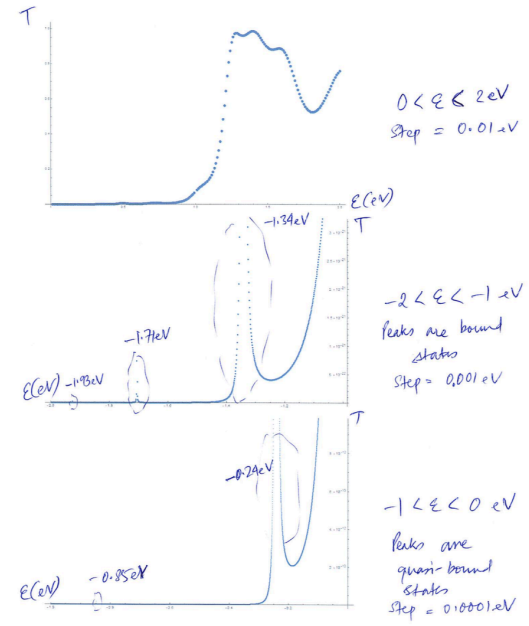


Figure 5•5–2. Barrier containing several flat-potential regions of varying lengths and heights.

Mathematica Code for Simulating transmission through barriers.

```
Clear[v,l,k,energy,P,F,M,len,e1,e2,estep,elen,tr];
e1=0;
e2=2;
estep=0.01;
elen=Floor[1+((e2-e1)/estep)];
len=5;
energy=ConstantArray[0,elen];
tr=ConstantArray[0,elen];
Do[{energy[[i]]=(e1+((i-1)*estep))*econv},{i,elen}];
Array[v,len];
Array[l,len];
Array[k,len];
Array[P,len-1];
Array[F,len-1];
econv=1.6*10^-19;
lconv=10^-9;
con=(1.05*10^-34)^2/(2*9.1*10^-31);
v[1]=0;
v[2]=1;
v[3]=-2;
v[4]=0;
v[5]=-1;
l[1]=0;
l[2]=1;
l[3]=2;
l[4]=3;
l[5]=0;
Do[{v[i]=v[i]*econv,l[i]=l[i]*lconv},{i,len}];
Do[{
    Do[{k[i1]=Sqrt[(energy[[j]]-v[i1])/con]},{i1,len}],
    M={{1,0},{0,1}},
    Do[{P[i-1]={{(k[i-1]+k[i])/(2*Sqrt[k[i-1]*k[i]]),(k[i-1]-k[i])/(2*Sqrt[k[i]*k[i-1]])},
               {(k[i-1]-k[i])/(2*Sqrt[k[i]*k[i-1]]),(k[i-1]+k[i])/(2*Sqrt[k[i-1]*k[i]])}},
       F[i-1]={{Exp[-I*k[i]*l[i]],0},{0,Exp[I*k[i]*l[i]]}},
       M=M.P[i-1].F[i-1]},{i,2,len}],
    tr[[j]]=1/Abs[M[[1,1]]^2],{j,elen}];
Do[{energy[[i]]=energy[[i]]/econv},{i,elen}];
ListPlot[Transpose[{energy,tr}]]
```

2.4) a)



$0 < E < 2$ eV
Step = 0.01 eV

$-2 < E < -1$ eV
Peaks are bound states
Step = 0.001 eV

$-1 < E < 0$ eV
Peaks are quasi-bound states
Step = 0.0001 eV

(b) [by Andrei & Sayak]

#6•4-1: Tunneling through a Barrier with an Applied Voltage

In solid-state physics, one encounters the problem of the tunneling of electrons through a thin oxide layer between two metals, as a function of the voltage ΔV applied between the metals. A simple model of this problem is the tunneling through the trapezoidal barrier shown in **Fig. 6.4–2**.

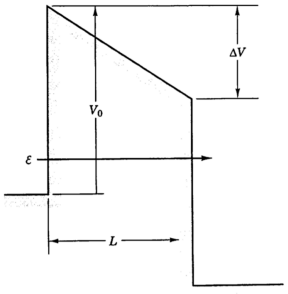
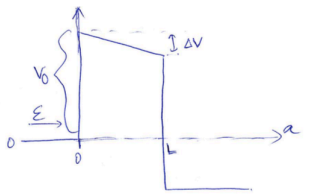


Figure 6•4–2. Trapezoidal barrier model for the tunneling of electrons through an oxide barrier between two metals.

Determine the tunneling probability as a function of ΔV, provided that ΔV remains less than $V_0 - \mathcal{E}$. For simplification, assume that L and V_0 are large enough that the total tunneling probability remains very small compared to unity.

2.4) b)



for $x<0$, $\psi_1(x) = \frac{A}{\sqrt{k_1}} e^{ik_1 x} + \frac{B}{\sqrt{k_1}} e^{-ik_1 x}$

$0<x<L$, $\psi_2(x) = \frac{C}{\sqrt{k_2(x)}} e^{\left(\int_0^x k_2(x)dx'\right)} + \frac{D}{\sqrt{k_2(x)}} e^{-\int_0^x k_2(x)dx'}$

$x>L$, $\psi_3(x) = \frac{F}{\sqrt{k_3}} e^{ik_3 x} + \frac{G}{\sqrt{k_3}} e^{-ik_3 x}$

$k_1 = \sqrt{\frac{2m}{\hbar^2}\varepsilon}$, $k_2(x) = \sqrt{\frac{2m}{\hbar^2}(V_0 - \frac{\Delta V x}{L} - \varepsilon)}$,

$k_3(x) = \sqrt{\frac{2m(\varepsilon+\Delta V)}{\hbar^2}}$

Now, the coefficients A & B are related to F & G by,

$$\begin{pmatrix} A \\ B \end{pmatrix} = \frac{1}{2\sqrt{k_1 k_2(0)}} \begin{pmatrix} k_1 + ik_2(0) & k_1 - ik_2(0) \\ k_1 - ik_2(0) & k_1 + ik_2(0) \end{pmatrix} \begin{pmatrix} e^{\int_0^L k_2(x)dx'} & 0 \\ 0 & e^{-\int_0^L k_2(x)dx'} \end{pmatrix}$$

$$\frac{1}{2i\sqrt{k_2(0)k_3}} \begin{pmatrix} k_3 + ik_2(L) & ik_2(L) - k_3 \\ ik_2(L) - k_3 & k_3 + ik_2(L) \end{pmatrix} \begin{pmatrix} F \\ G \end{pmatrix}$$

1st matrix is for step at $x=0$, 2nd is for propagation through the barrier, 3rd is for step at $x=L$.

$$\Rightarrow \begin{pmatrix} A \\ B \end{pmatrix} = \begin{pmatrix} M_{11} & M_{12} \\ M_{21} & M_{22} \end{pmatrix} \begin{pmatrix} F \\ G \end{pmatrix}$$

For transmission coefficient, $T = \frac{|F|^2}{|A|^2} = \frac{1}{|M_{11}|^2}$

We define $\alpha = \exp\left[\int_0^L k_2(x)dx'\right]$

So, $|M_{11}|^2 = \frac{1}{16 k_1 k_3 k_2(0) k_2(L)} \left[\left(\alpha - \frac{1}{\alpha}\right)^2 \left(k_1 k_3 - k_2(0) k_2(L)\right)^2 + \left(\alpha + \frac{1}{\alpha}\right)^2 \left(k_1 k_2(L) + k_2(0) k_3\right)^2\right]$

For $V_0 >> \Delta V$ and large L, T is low ($<<1$).

In this condition, $\alpha >> 1/\alpha$

$$|M_{11}|^2 \approx \frac{\alpha^2}{16 k_1 k_3 k_2(0) k_2(L)} (k_1^2 + k_2^2(0))(k_3^2 + k_2^2(L))$$

$$= \frac{\alpha^2 (\varepsilon + V_0 - \varepsilon)(\varepsilon + \Delta V + V_0 - \varepsilon - \Delta V)}{16\sqrt{\varepsilon(\varepsilon+\Delta V)}(V_0 - \varepsilon)(V_0 - \varepsilon - \Delta V)}$$

$$\approx \frac{\alpha^2 V_0^2}{16\sqrt{\varepsilon(\varepsilon+\Delta V)}(V_0 - \varepsilon)}$$

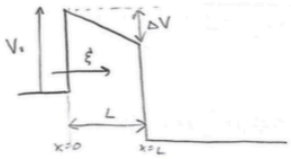
$$\alpha = \exp\left[\int_0^L \sqrt{\frac{2m}{\hbar^2}} \sqrt{V_0 - \frac{\Delta V x'}{L} - \varepsilon}\, dx'\right]$$

$$\therefore T = \frac{1}{|M_{11}|^2} = \boxed{\frac{16(V_0 - \varepsilon)}{\alpha^2 V_0^2}\sqrt{\varepsilon(\varepsilon+\Delta V)}}$$

$$\boxed{T(\varepsilon) = \frac{16(V_0 - \varepsilon)\sqrt{\varepsilon(\varepsilon+\Delta V)}}{V_0^2} \cdot e^{-2\int_0^L \sqrt{\frac{2m}{\hbar^2}\left(V_0 - \frac{\Delta V x'}{L} - \varepsilon\right)}\, dx'}}$$

And the WKB tunneling probability integral is given by:

b) Kroemer 6.4-1 ; Tunneling through a barrier w/ applied voltage



$\Delta V < V_0 - \varepsilon$

Using WKB approximation.

$$T_{WKB} \approx \exp\left[-2\int_0^L dx \sqrt{\frac{2m}{\hbar^2}\left[E_c(x) - \varepsilon\right]}\right]$$

$$E_c(x) = -\frac{\Delta V}{L} x + V_0$$

$$T_{WKB} = \exp\left[-2\int_0^L dx \sqrt{\frac{2m}{\hbar^2}\left(-\frac{\Delta V}{L} x + V_0 - \varepsilon\right)}\right]$$

$$\text{Int} = \sqrt{\frac{2m}{\hbar^2}} \cdot \left(\frac{-1}{\Delta V}\right) \cdot \int_0^L dx \sqrt{\frac{-\Delta V}{L} x + V_0 - \varepsilon} = \sqrt{\frac{2m}{\hbar^2}} \cdot \left[\frac{2}{3}\left(-\frac{\Delta V}{L} x + V_0 - \varepsilon\right)^{3/2}\right]_0^L$$

$u = -\frac{\Delta V}{L} x + V_0 - \varepsilon$

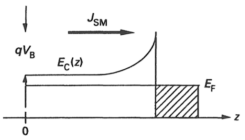
$du = -\frac{\Delta V}{L} dx$

$$= \sqrt{\frac{2m}{\hbar^2}} \cdot \frac{2}{3} \cdot \left((V_0 - \Delta V - \varepsilon)^{3/2} - (V_0 - \varepsilon)^{3/2}\right)$$

$$\boxed{T(\Delta V, \varepsilon) = \exp\left[-\frac{4}{3} \cdot \sqrt{\frac{2m}{\hbar^2}}\left[(V_0 - \Delta V - \varepsilon)^{3/2} - (V_0 - \varepsilon)^{3/2}\right]\right]}$$

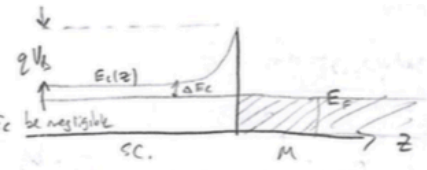
(c) [solution by Andrei, and further detailed solution from ece4070/mse 6050]

1.15 Consider a metal-semiconductor barrier as shown below:



(a) Write an expression, involving a sum, for the electron current injected from the semiconductor to the metal, J_{SM}.
(b) Convert the sum to an integral. Be sure to show the limits of integration.
(c) Sketch the transmission coefficient versus k_z expected from (1) quantum mechanical and (2) classical considerations.
(d) Set up the problem for computing the classical (thermionic emission) current J_{SM}. Show the formula that has to be integrated, but do not integrate it.
(e) Evaluate the integral and show that the result is the expected thermionic emission relation.

c) Lundstrom 1.15



Schottky

let $g_s = g_v = 1$

a) $J_{SM} = q \sum_k \vec{v}_g(\vec{k}) \cdot f(k)$ where $v_g = \frac{1}{\hbar}\frac{dE_c(z)}{dz}$ $\quad f(k_z) = \frac{1}{1+\exp\left[\frac{\frac{\hbar^2 k_z^2}{2m^*_c} - E_F}{k_B T}\right]}$

$$J_{SM} = \frac{q}{\hbar}\sum_{k_z}\frac{dE_c(z)}{dz} f(k_z)$$

b) $$J_{SM} = \frac{q}{\hbar(2\pi)}\int_{k_{z_0}}^{\infty} dk_z \frac{\delta E_c(z)}{dz} f(k_z)$$

let $E_c(z=0) = \frac{\hbar^2 k_{z_0}^2}{2m^*_c} = E_F$ assume parabolic band structure.

k_{z_0}

$k_{zB} \rightarrow \frac{\hbar^2 k_{zB}^2}{2m^*_c} = E_F + qV_B$

c) $T(k_z)$ for QM and classical.

d) Classically, can't tunnel only $\frac{\hbar^2 K^2}{2m^*_c} > qV_B + E_F$

$J_{SM} = \int q\, n(E)\, v_z(E)\, dE$

where $n(E)dE = f(E)\, g_c(E)\, dE = \frac{8\pi\sqrt{2}}{h^3}\cdot m^{*}\cdot \frac{\sqrt{E}\,dE}{1+\exp\left[\frac{E-E_F}{k_B T}\right]}$ (conduction)

electron velocity: $E = \frac{mv^2}{2} \rightarrow \sqrt{E}\,dE = \frac{m^{3/2}}{\sqrt{2}} v^2\, dv$

$\hookrightarrow n(E)dE = \frac{8\pi m^3}{h^3}\frac{v^2 dv}{1+\exp\left[\frac{E-E_F}{k_B T}\right]} \simeq \frac{2m^3}{h^3}\exp\left[-(E-E_F)/k_B T\right] 4\pi v^2\, dv$

$qV_B - E_F > 3k_B T$

Now, $E = \frac{mv^2}{2} = \frac{m}{2}\left(v_x^2 + v_y^2 + v_z^2\right)$

$$J_{SM} = \frac{2qm^3}{h^3}\exp\left[E_F/k_B T\right]\int_{v_{x\min}}^{\infty} v_x \exp\left[\frac{-mv_x^2}{2k_B T}\right]dv_x \int_{-\infty}^{\infty}\exp\left[\frac{-mv_y^2}{2k_B T}\right]dv_y \int_{-\infty}^{\infty}\exp\left[\frac{-mv_z^2}{2k_B T}\right]dv_z$$

$v_{x\min} \rightarrow E_{\min} = E_F + qV_B = \frac{m v_{x\min}^2}{2} \rightarrow v_{x\min} = \left(\frac{2}{m}(E_F + qV_B)\right)^{1/2}$

e) Evaluating the above integral,

$$J_{SM} = \frac{k_B^2 m \pi q}{h^3}\exp\left[-\frac{(E_F + qV_B)}{k_B T}\right]\cdot T^2$$

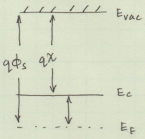
which is of the form $J = A_R T^2 \exp\left[-\frac{qV_B}{k_B T}\right]$

which is the expected thermionic emission relation.

(a) Work function of a semiconductor is the difference between the vaccum level and fermi energy.

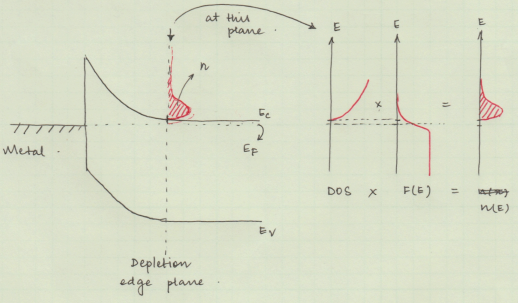
$$q\Phi_s = q\chi + (E_c - E_F)$$

Φ_s : Work fn. of semicond
χ : electron affinity



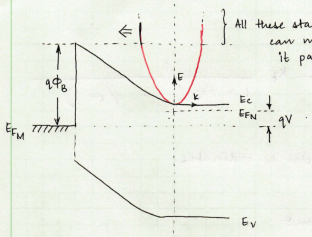
There is a depletion region formed in the metal - semiconductor junction region since the two have different fermi levels to begin with. In order to come to equilibrium with each other, the Fermi Levels need to match up, which can be achieved by the movement of the mobile charges. This leaves behind the +ve charged dopants, forming a depletion region.

(b)



(c) Consider a bias V being applied now.

Which means the fermi levels in the metal & semiconductor aren't lined up, but separated by qV.



Looking at the band diagram / structure, we can see that only those k-states with Energy more than the barrier height will get through.

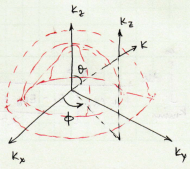
$$\therefore E(k) > q\Phi_B - (E_c - E_{FN}) - (E_{FN} - E_{FM})$$

$$\frac{\hbar^2}{2m^*}(k_x^2 + k_y^2 + k_z^2) > q\Phi_B - (E_c - E_{FN}) - qV$$

$$\therefore \Omega_k \left\{ k_x^2 + k_y^2 + k_z^2 > \frac{2m_c^*}{\hbar}\left(q\Phi_B - (E_c - E_{FN}) - qV\right) \right\}$$

(d) Now, we calculate the current going through (over) the barrier.

We want the current in the z-direction only.



z-dir. Current due to k-state.

$$J_k = q\frac{g_s g_v}{L^3}\left(\vec{v_g}\cdot\hat{z}\right) f(k)$$

group velocity in $\hat{z}$

$$J(k) = q\,\frac{g_s g_v}{L^3}\,\frac{\hbar k_z}{m_c^*}\cdot\frac{1}{1+\exp\left(\left(E_c+\frac{\hbar^2}{2m_c^*}(k_x^2+k_y^2+k_z^2)-E_{FM}\right)/kT\right)}$$

going left (semi-to-metal).

∴ Net current can be obtained by integrating over k-in the not. prev. obtained Ω_k.

$$J_{\leftarrow} = q\,\frac{g_s g_v \hbar}{m_c^*}\int_{\Omega_k}\frac{dk_x\,dk_y\,dk_z}{(2\pi)^3}\,k_z\cdot\frac{1}{1+\exp\left(\cdot\,/kT\right)}$$

we can go into polar co-ordinates

$k_z = k\cos\theta$

$k_x = k\cos\phi\sin\theta$

$k_y = k\sin\phi\sin\theta$

Ω_k : $k_x^2+k_y^2+k_z^2 \Rightarrow k > \sqrt{\frac{2m_c^*}{\hbar^2}(q\phi_b-(E_c-E_{FN})-qV}$ $= k_{min}$

$k > k_{min}$

Integral changes to :

$$J_{\leftarrow} = q\,\frac{g_s g_v \hbar}{(2\pi)^3 m_c^*}\int (k^2\sin\theta\,dk\,d\theta\,d\phi)(k\cos\theta)\,\frac{1}{1+\exp\left[\frac{E_c-E_{FN}+\frac{\hbar^2k^2}{2m^*}}{kT}\right]}$$

$k : k_{min} \to \infty$

$\theta : 0 \to 2\pi$

$\phi : 0 \to \pi/2$

$$= q\,\frac{g_s g_v \hbar}{(2\pi)^3 m_c^*}(2\pi)\int_{\theta=0}^{\pi/2} d\theta\,\sin\theta\cos\theta \cdot \int_{k_{min}}^{\infty} dk\,\frac{k^3}{1+\exp\left[\frac{E_c-E_{FN}+\hbar^2k^2/2m^*}{kT}\right]}$$

$\pi/2$ → ½

for the second integral in dk, we can apply the Maxwell Boltzmann approx :

$$J_{\leftarrow} = \frac{q\,g_s g_v \hbar}{(2\pi)^2\cdot m_c^*\cdot 2}\int_{k_{min}}^{\infty} dk\cdot k^3\, e^{-(E_c-E_{FN})/kT}\, e^{-\hbar^2k^2/2m^*kT}$$

$$= q\,\frac{g_s g_v \hbar}{8\pi^2 m_c^*}\, e^{-(E_c-E_{FN})/kT}\int_{k_{min}}^{\infty} dk\cdot k^3\cdot e^{-\hbar^2k^2/2m^*kT}$$

(use mathematica)

$$= q\,\frac{g_s g_v \hbar}{8\pi^2 m_c^*}\, e^{-(E_c-E_{FN})/kT}\cdot\frac{1}{2}\left(\frac{2m_c^*kT}{\hbar^2}\right)^2\left\{\frac{2m_c^*}{\hbar^2}(kT+q\phi_B-(E_c-E_F)-qV\right\}$$

$$e^{-\left\{\frac{\hbar^2}{2m^*kT}\cdot\frac{2m^*}{\hbar^2}\cdot[q\phi_B-(E_c-E_{FN})-qV]\right\}}$$

$$= \frac{q\,g_s g_v\, m_c^*}{4\pi^2\hbar^3}(k_BT)^2\left\{kT+q\phi_B-(E_c-E_{FN})-qV\right\}e^{-(q\phi_B-qV/kT)}$$

$$= \frac{q\,g_s g_v\, m_c^* k_B^2}{4\pi^2\hbar^3}\cdot T^2\left\{1+\eta\right\}e^{-q\phi_B}\cdot e^{+qV/kT}$$

$$J_{\leftarrow} = A^*T^2 e^{-q\phi_B}e^{+qV/kT}\cdot \quad ; \text{ where, } A^* = \frac{q\,g_s g_v\, m_c^* k_B^2}{4\pi^2\hbar^3}(1+\eta)$$

$$\eta = \frac{q\phi_B-(E_c-E_{FN})-qV}{k_BT}$$

Remember, this is just the current going left (from the semi-conductor to metal).

for the right going carriers, fermi energy = fermi energy of the metal E_{FM}.

∴ they won't see the voltage $qV = E_{FN} - E_{FM}$.

∴ By symmetry, we can divine ;

$$J_{\rightarrow} = -A^*T^2e^{-q\phi_B}\cdot e^0 = -A^*T^2e^{-q\phi_B}$$

(-ve sign since it is in opp. direction and we take proj of v_g along z in our expression)

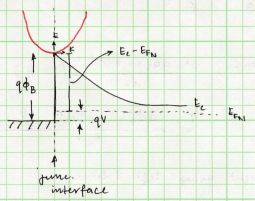
∴ Net current = $J_{net} = |J_{\rightarrow}| - |J_{\leftarrow}|$

$$J_{net} = A^*T^2e^{-q\phi_B}\left(e^{+qV/k_BT}-1\right)$$

(c) for $\eta \to 0$ (diffusive limit), $J = J_s\left(e^{qV/kT}-1\right)$

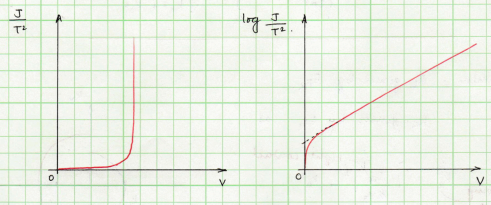
Since we are considering the case where only the carriers close to the junction will make it past (diffuse) to the metal, at that interface plane

$(E_c - E_{FN}) + qV$ ≈ Barrier height ≈ $q\phi$ (slightly less than)



∴ $\eta \to 0$

(f) Plots attached



The general shapes of the curves are shown.

The y-intercept of the log plot can be used to measure m_c^*.

$$\frac{J}{T^2} = \frac{4\pi q k_B^2 m_c^*}{h^3}\, e^{-q\phi_B/kT}\left(e^{qV/k_BT}-1\right)$$

in the linear regn. of the log plot : $e^{qV/k_BT} \gg 1$

$$\ln\left(J/T^2\right) = \ln\left\{\frac{4\pi q k_B^2}{h^3}\cdot m_c^*\, e^{q(-\phi_B+V)/kT}\right\}$$

$$= q(-\phi_B+V)/kT + \ln\left\{\frac{4\pi q k_B^2}{h^3}\cdot m_c^*\right\}$$

$$= \left(\frac{q}{kT}\right)V + -\phi_B q + \ln\left\{(\,\cdot\,)m_c^*\right\}$$

↳ $y = mx + c$

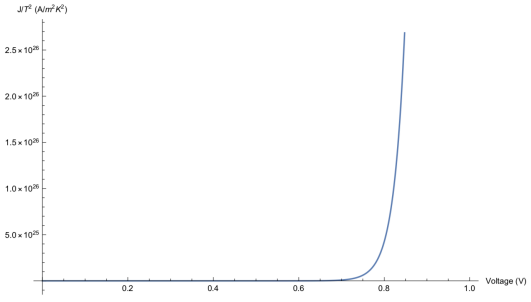
∴ the y-intercept is :

$$-\phi_B q + \ln\left\{\frac{4\pi q k_B^2}{h^3}\cdot m_c^*\right\}$$, where all are fundamental constants except ϕ_B & m_c^*.

∴ Knowing one will give us the other experimentally.

```
In[965]:= ClearAll["Global`*"] (* Clear all variables *)

qe = 1.6 * 10^-19;
ħ = 6.63/(2 π) * 10^-34;
kb = 1.38 * 10^-23;
me = 9.1 * 10^-31;
mcGaAs = 0.067;

aStar = qe * 4 π * me * kb * 0.067 * mcGaAs / ħ^3;
T = 300;
jbyTsq[voltage_] := aStar * Exp[-qe/(kb * T)] * (Exp[qe * voltage/(kb * T)] - 1);
yintercept[voltage_] := aStar * Exp[-qe/(kb * T)] * Exp[qe * voltage/(kb * T)];

Plot[jbyTsq[v], {v, 0, 1},
 AxesLabel → {"Voltage (V)", "J/T² (A/m²K²)"}, ImageSize → Large]
LogPlot[{jbyTsq[v], yintercept[v]}, {v, 0, 1},
 AxesLabel → {"Voltage (V)", "Log (J/T²) (A/m²K²)"},
 ImageSize → Large, PlotStyle → {Automatic, {Red, Dashed}}]

yintercept[0] (*Finding the y-intercept from the log plot*)
```

Out[974]=



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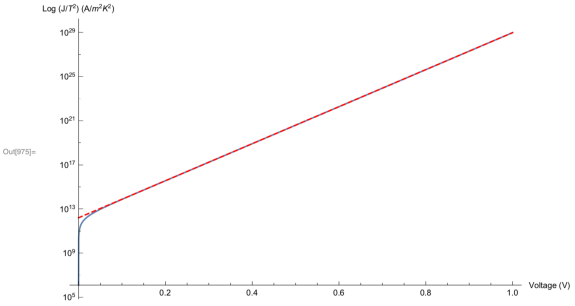


Problem 2.5: A 2DEG as a parallel array of 1D conductors

Here is a question from the 2017 ECE 4070/MSE 6050 Final exam. It is very relevant for this class. Electrons of sheet carrier density n_s sit in the conduction band of a 2D electron system of energy bandstructure $E(k_x, k_y) = \frac{\hbar^2}{2m_c^*}(k_x^2 + k_y^2)$ with the $k-$space occupation of carriers shown in Figure 1. The grey shaded states are occupied, rest are empty. Assume a spin degeneracy of $g_s = 2$ and a valley degeneracy of $g_v = 1$. The width of the 2D system is W, the length L, and ohmic source and drain contacts are made to connect to the electrons to flow a current in the $x-$direction. Solve this problem entirely at $T = 0$ K. The allowed discrete points in the $k-$space $(k_x, k_y) = (\frac{2\pi}{L}n_x, \frac{2\pi}{W}n_y)$ where (n_x, n_y) are integers are considered individual *modes* of the 2DEG as indicated in Figure 1. The collection of modes with the same n_y is considered a 1D mode of the 2DEG.

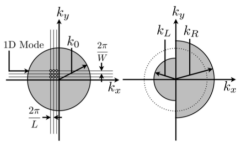


Figure 1: Lateral Modes of a 2D Electron System.

(a) When the applied voltage across the source/drain contacts is $V_{ds} = 0$, find the Fermi wavevector k_0 as shown in the left of Figure 1.

(b) Show that the number of 1D modes with current flow in the x-direction because of the finite width of the 2D conductor is $M_0 = \frac{k_0 W}{\pi}$. Use part (a) to write this in terms of the 2DEG density.

(c) Now a voltage V_{ds} is applied across the drain and the source such that the net sheet carrier density of the 2DEG does not change. Assume ballistic transport and show that in Figure 1, $k_R = \sqrt{k_0^2 + \frac{m_c^*}{\hbar^2}(qV_{ds})}$ and $k_L = \sqrt{k_0^2 - \frac{m_c^*}{\hbar^2}(qV_{ds})}$.

(d) Show that the voltage V_{ds} reduces the total number of left going modes M_L and increases the total number of right going modes M_R. Find expressions for M_L and M_R.

(e) Find the voltage V_{ds} at which carriers in all modes move to the right and no carriers move to the left.

(f) Find how many right-going 1D modes are present in the above situation when all carriers move to the right.

(g) Because each 1D mode in the ballistic limit can provide the maximum conductance of a quantum of conductance $G = \frac{g_s g_v q^2}{h}$, find the 'saturation' current I_d when the critical V_{ds} of part (e) is reached.

Solution:[From ECE 4070/MSE 6040 2016]

carrier density : n_s ; $E(k_x, k_y) = \frac{\hbar^2}{2m_c^*}(k_x^2 + k_y^2)$

$g_s = 2$; $g_v = 1$ ✓

(a) carrier density · area = # of k states × $g_s g_v$

$E_F = \frac{\hbar^2}{2m_c^*}(k_0^2)$

$k \cdot W \cdot n_s = \frac{\pi \cdot k_0^2}{\left(\frac{2\pi}{L}\right)\left(\frac{2\pi}{W}\right)} \cdot g_s g_v$

$n_s = \frac{k_0^2}{4\pi} g_s g_v$

$|k_0| = \left(\frac{4\pi n_s}{g_s g_v}\right)^{1/2} = \boxed{(2\pi n_s)^{1/2}}$ ✓

(b) The Fermi wavevector k_0 shows the maximum k.

The distance in x-direction is $\frac{2\pi}{W}$

The number of 1D modes would be $\frac{k_0}{\frac{2\pi}{W}} \cdot 2$ ← from $-k_0$ to k_0

$M = \frac{k_0 W}{\pi}$ ✓

$\boxed{M_0 = \frac{(2\pi n_s)^{1/2} \cdot W}{\pi}}$ ✓

(c) $E_R - E_L = q V_{ds}$

$E_F = \frac{\hbar^2}{2m_c^*} k_0^2$

$E_R = E_F + \frac{1}{2} q V_{ds} \Rightarrow \frac{\hbar^2}{2m_c^*} k_R^2 = \frac{\hbar^2}{2m_c^*} k_0^2 + \frac{1}{2} q V_{ds}$

$\boxed{k_R = \sqrt{k_0^2 + \frac{m_c^*}{\hbar^2}(q V_{ds})}}$ ✓

Similarly, $k_L = \sqrt{k_0^2 - \frac{m_c^*}{\hbar^2}(q V_{ds})}$ ✓

Show that n_s doesn't change

(d) $M_R = \frac{k_R \cdot W}{\pi} \times 2$ $M_L = \frac{k_L \cdot W}{\pi} \times 2$ ← since $2k_L$ $2k_R$.

$M_R = \frac{\sqrt{k_0^2 + \frac{m_c^*}{\hbar^2}(q V_{ds})} \cdot W}{\pi}$ ✓ $M_L = \frac{\sqrt{k_0^2 - \frac{m_c^*}{\hbar^2}(q V_{ds})} \cdot W}{\pi}$ ✓

When V_{ds} ↑, k_R ↑, M_R ↑, but k_L ↓, M_L ↓

(e) To reach this state, $k_L = 0$

$k_L = \sqrt{k_0^2 - \frac{m_c^*}{\hbar^2}(q V_{ds})} = 0$

$k_0^2 = \frac{m_c^*}{\hbar^2}(q V_{ds})$

$2\pi n_s = \frac{m_c^*}{\hbar^2}(q V_{ds})$

$\boxed{V_{ds} = \frac{2\pi \hbar^2 n_s}{q m_c^*}}$ ✓

(f) $k_R = \sqrt{k_0^2 + \frac{m_c^*}{\hbar^2}(q V_{ds})} = k_0 \cdot \sqrt{2}$ ✓

$M_R = \frac{k_R \cdot W}{\pi} = \frac{k_0 \cdot \sqrt{2} \cdot W}{\pi} = \frac{k_0 \cdot W \sqrt{2}}{\sqrt{2} \cdot \pi}$

$= \frac{\sqrt{2\pi n_s} \cdot W}{\sqrt{2} \cdot \pi} = \boxed{2\sqrt{\frac{n_s}{2\pi}} \cdot W}$ ✓

(g) For each 1D mode, $G = \frac{g_s g_v \cdot q^2}{h}$

$I = G \cdot V$

$I_d = M_R \cdot G \cdot V_{ds}$

$= 2\sqrt{\frac{n_s}{\pi}} \cdot W \cdot \frac{2q^2}{h} \cdot \frac{2\pi \hbar^2 n_s}{q m_c^*}$

$= \boxed{\frac{1}{\sqrt{\pi}} \cdot \frac{4W q \cdot \hbar \cdot (n_s)^{3/2}}{m_c^*}}$

Problem 2.6: A Ballistic FET with a 2D Semiconductor Crystal

Problem 2.6) A Ballistic FET with a 2D Semiconductor Crystal
We derived the characteristics of a ballistic field-effect transistor in class. Assume a double-gated 2D semiconductor crystal (e.g. MoS_2) with a gate barrier thickness $t_b = 4$nm, and a dielectric constant $\epsilon_b = 20\epsilon_0$.

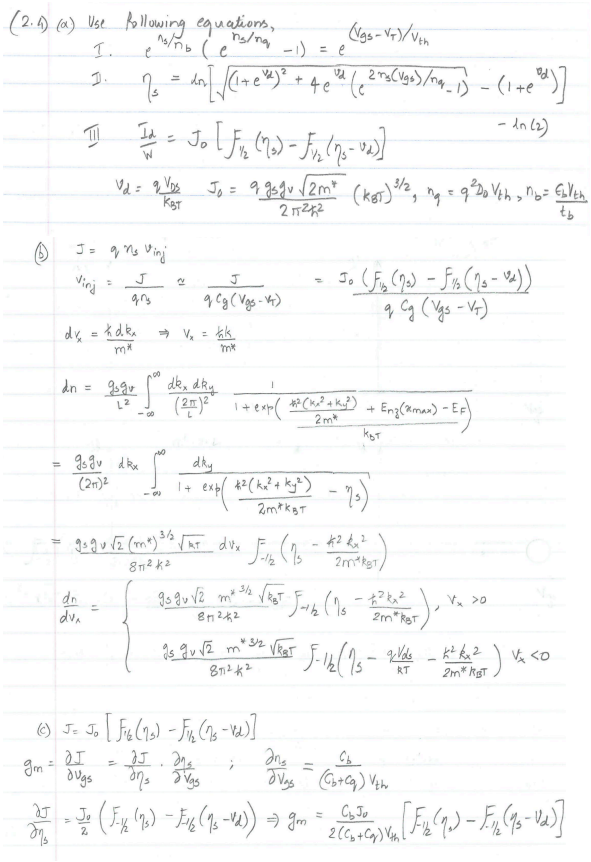
(a) Plot the 77K and 300K $I_d - V_{ds}$ and $I_d - V_{gs}$ characteristics of the 2D crystal FETs made of a semiconductor with dispersion $E(k) = \hbar^2 k^2/2m^\star$ with $m^\star = 0.3m_0$. Use a spin degeneracy of $g_s = 2$ and a valley-degeneracy of $g_v = 1$. Compare the characteristics of the transistor for a 2D crystal semiconductor with $m^\star = 0.2m_0$.

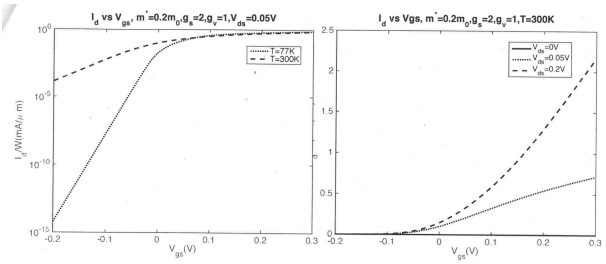
(b) Find an expression for the effective carrier injection velocity v_{inj} by writing the current per unit width as $I_d = qn_s v_{inj}$ where $n_s \sim C_g(V_{gs} - V_T)$ in the on-state of the ballistic FET. Make plots for the parameters in part (a). Note that not all the n_s carriers are *actually* moving at uniform velocity of v_{inj}. Make a 'spectral' plot of the number of carriers vs the velocity in the direction of the source/drain contacts, that runs from -ve to +ve velocities, for 77K and for 300K for the parameters for part (a).

(c) Find expressions for the gain (transconductance per unit width, $g_m = \frac{\partial I_d}{\partial V_{gs}}$) for the ballistic FET as a function of the gate voltage V_{gs} and small $V_{ds} << kT/q$, and for V_{ds} in current saturation. Make plots for the parameters of part (a) and comment.

(d) A popular method to extract the field-effect mobility in FETs in the 'resistor' or linear region of operation where the electric field driving transport is $F \sim V_{ds}/L$ is the following: For a channel length L use $qn_s \sim C_b(V_{gs} - V_T)$ with the drift current per unit width $I_d = qn_s\mu\frac{V_{ds}}{L}$ to write $I_d = C_b(V_{gs} - V_T)\mu\frac{V_{ds}}{L}$, and take the slope of the measured $I_d - V_{gs}$ curve to extract μ. Because C_b, V_{ds} and L are precisely known, this gives the unknown μ. Find an expression for the effective 'mobility' that will be measured when this technique is applied to a *ballistic* FET, and why the results must not be trusted.

Solution: [By Wenshen, 2015] Note: This solution uses a different effective mass, but the answers and trends are the same.

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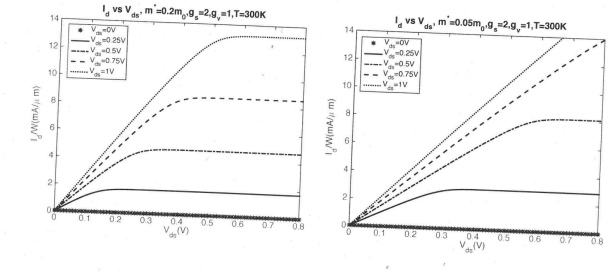
T=77K
T=300K
V_gs(V)


I_d vs Vgs, m*=0.2m_0,g_s=2,g_v=1,T=300K
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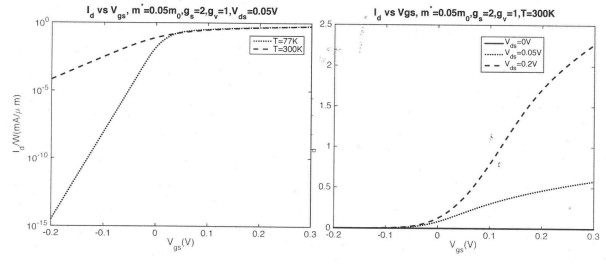
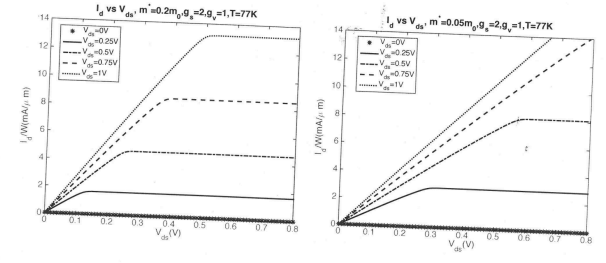
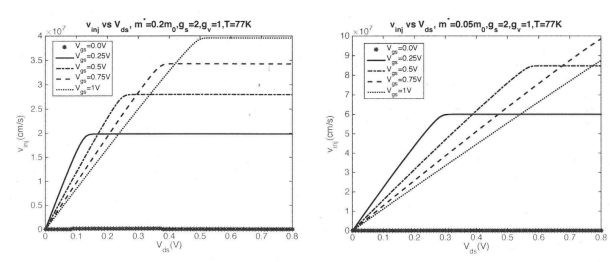
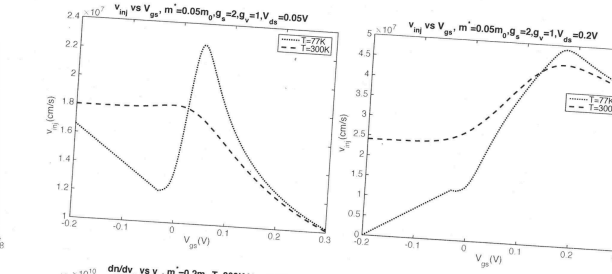
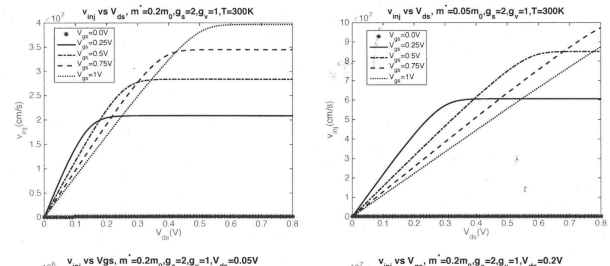
V_ds=0.05V
V_ds=0.2V
V_gs(V)

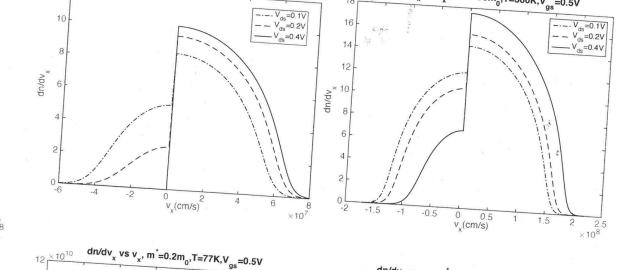

I_d vs V_gs, m*=0.05m_0,g_s=2,g_v=1,V_ds=0.05V
T=77K
T=300K
V_gs(V)


I_d vs Vgs, m*=0.05m_0,g_s=2,g_v=1,T=300K
V_ds=0V
V_ds=0.05V
V_ds=0.2V
V_gs(V)


v_inj vs V_ds, m*=0.2m_0,g_s=2,g_v=1,T=77K
V_gs=0.0V
V_gs=0.25V
V_gs=0.5V
V_gs=0.75V
V_gs=1V
V_ds(V)


v_inj vs V_ds, m*=0.05m_0,g_s=2,g_v=1,T=77K
V_gs=0.0V
V_gs=0.25V
V_gs=0.5V
V_gs=0.75V
V_gs=1V
V_ds(V)


v_inj vs V_ds, m*=0.2m_0,g_s=2,g_v=1,T=300K
V_gs=0.0V
V_gs=0.25V
V_gs=0.5V
V_gs=0.75V
V_gs=1V
V_ds(V)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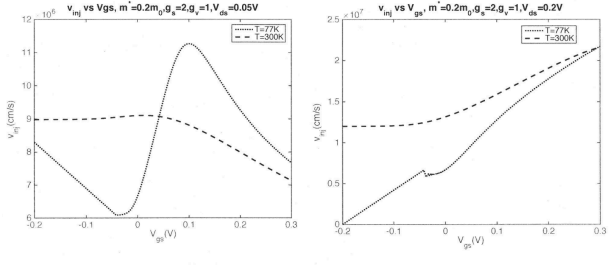
V_gs=0.0V
V_gs=0.25V
V_gs=0.5V
V_gs=0.75V
V_gs=1V
V_ds(V)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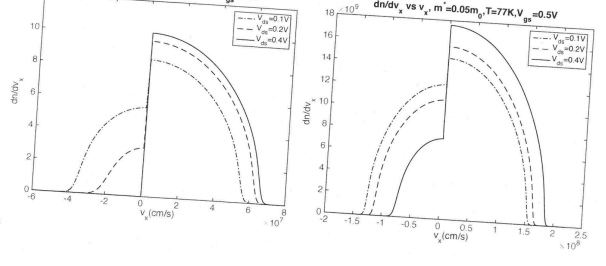
T=77K
T=300K
V_gs(V)


v_inj vs V_gs, m*=0.2m_0,g_s=2,g_v=1,V_ds=0.2V
T=77K
T=300K
V_gs(V)

v_inj vs V_gs, m*=0.05m_0,g_s=2,g_v=1,V_ds=0.05V
T=77K
T=300K
V_gs(V)

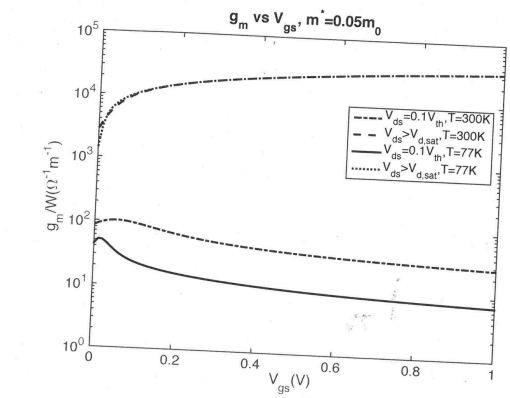
v_inj vs V_gs, m*=0.05m_0,g_s=2,g_v=1,V_ds=0.2V
T=77K
T=300K
V_gs(V)

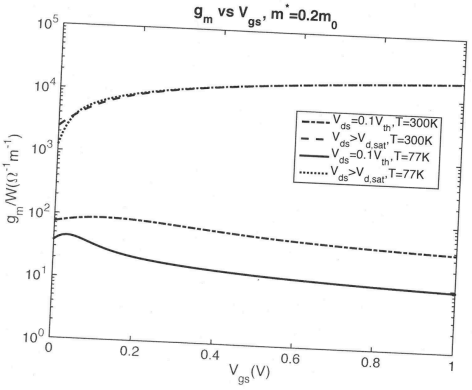
dn/dv_x vs v_x, m*=0.2m_0,T=300K,V_gs=0.5V
V_ds=0.1V
V_ds=0.2V
V_ds=0.4V
v_x(cm/s)

dn/dv_x vs v_x, m*=0.05m_0,T=300K,V_gs=0.5V
V_ds=0.1V
V_ds=0.2V
V_ds=0.4V
v_x(cm/s)

dn/dv_x vs v_x, m*=0.2m_0,T=77K,V_gs=0.5V
V_ds=0.1V
V_ds=0.2V
V_ds=0.4V
v_x(cm/s)

dn/dv_x vs v_x, m*=0.05m_0,T=77K,V_gs=0.5V
V_ds=0.1V
V_ds=0.2V
V_ds=0.4V
v_x(cm/s)


g_m vs V_{gs}, $m^*=0.05m_0$
$g_m/W(\Omega^{-1}m^{-1})$
V_{gs}(V)
$V_{ds}=0.1V_{th}$,T=300K
$V_{ds}>V_{d,sat}$,T=300K
$V_{ds}=0.1V_{th}$,T=77K
$V_{ds}>V_{d,sat}$,T=77K


g_m vs V_{gs}, $m^*=0.2m_0$
$g_m/W(\Omega^{-1}m^{-1})$
V_{gs}(V)
$V_{ds}=0.1V_{th}$,T=300K
$V_{ds}>V_{d,sat}$,T=300K
$V_{ds}=0.1V_{th}$,T=77K
$V_{ds}>V_{d,sat}$,T=77K