ECE 5390/MSE 5472, Fall Semester 2017
Quantum Transport in Electron Devices & Novel Materials

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Assignment 2

Policy on assignments: Please turn them in by 5pm of the due date. The due date for this assignment is **Monday, Oct 2nd, 2017**.

General notes: Present your solutions *neatly*. Do not turn in rough unreadable worksheets - learn to **take pride in your presentation**. Show the relevant steps, so that partial points can be awarded. $\boxed{\text{BOX}}$ your final answers. Draw figures wherever necessary. Please print out this question sheet and staple to the top of your homework. Write your name and email address on the cover. Some problems may lead to publishable results - be on the lookout!

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.

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 $\{c_i, c_j^\dagger\} = c_i cj^\dagger + c_j^\dagger c_i = \delta_{ij}$ 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.

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.

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.

Problem 2.6) 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 $E(k_x, k_y) = \frac{\hbar^2}{2m_c^\star}(k_x^2 + k_y^2)$ 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.

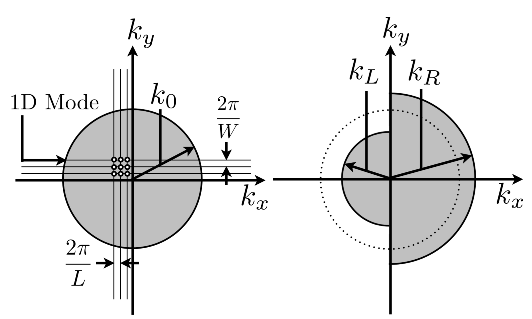

Figure 1: Lateral Modes of a 2D Electron System.

(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, $k_R = \sqrt{k_0^2 + \frac{m_c^\star}{\hbar^2}(qV_{ds})}$ and $k_L = \sqrt{k_0^2 - \frac{m_c^\star}{\hbar^2}(qV_{ds})}$.

(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.

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 $m^\star = 0.3 m_0$. 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 $m^\star = 0.2 m_0$.

(b) Find an expression for the effective carrier injection velocity v_{inj} by writing the current per unit width as $I_d = q n_s v_{inj}$ 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 $q n_s \sim C_b(V_{gs} - V_T)$ with the drift current per unit width $I_d = q n_s \mu \frac{V_{ds}}{L}$ 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.