Problem set for the course "Theoretical Nanophysics" (2019 Spring)

Deadline: 21. June, 5pm. Please,do not send photos, use a proper scanner, or a mobile application such as CamScan to send us solutions.

Rules:

1. You can collect up to 30 points at maximum from each section
2. You can choose any number of problems within a section, but you cannot chose two problems with the same main number.
3. You are allowed to discuss with others and get help from each other, you can also consult us, lecturers, in case you are stuck, but you are supposed to hand in your own work.

Grading is as follows: 2: 31-40 points; 3: 41-55 points; 4: 56-70 points; 5: 71- points.

I. RANDOM MATRIX THEORY

1.1 (15pts) Wigner distribution for 2x2 unitary matrices: Consider a general 2x2 Hamiltonian, and parametrize it in terms of the Pauli matrices σ_0 (identity) and $\sigma_{x,y,z}$: $H = \sum_\alpha \Delta_\alpha \sigma_\alpha$. Construct the distance, $\mathrm{d}s^2 = \mathrm{Tr}(\mathrm{d}H\mathrm{d}H)$, from that the metric tensor, and show that the invariant measure is $\mathrm{d}\mu(H) = C\prod_\alpha \mathrm{d}\Delta_\alpha$. Express the eigenvalues in terms of these parameters, and also express the full Gaussian unitary distribution, $\propto \mathrm{d}\mu(H)e^{-\lambda \mathrm{Tr}(H^2)}$ in terms of these four real parameters. Next, introduce spherical coordinates (Δ, θ, and ϕ) for the parameters $\Delta_{x,y,z}$, compute the Jacobian, and reexpress the distribution in terms of these Gaussian variables. Integrate over the variables θ, ϕ, and Δ_0, and obtain the distribution of Δ. Finally, determine the average level spacing, $\delta\epsilon \equiv 2\langle\Delta\rangle$, and derive the distribution of the dimensionless level spacing, $s \equiv 2\Delta/\delta\epsilon$.

1.2 (25pts) Wigner distribution for a symplectic manyfold:

a. **(10pts)** Assume a two-level system with two spin degenerate levels, $|a\sigma\rangle$ and $|b\sigma\rangle$. Time reversal symmetry is represented by an anti-unitary operator, which satisfies the following relations: (1) It leaves the Hamiltonian invariant, $THT^\dagger = H$. (2) $T^2 = -1$. (3) $T|a\uparrow\rangle = |a\downarrow\rangle$ and $T|a\downarrow\rangle = -|a\uparrow\rangle$. (Similar relations hold for the other state). Starting from these properties and the requirement that the Hamiltonian matrix must be Hermitian show that the most general 4x4 matrix describing our two-level system is:

$$\mathbf{H} = \begin{pmatrix} \epsilon_a \mathbf{1} & \alpha_0\mathbf{1} + i\vec{\alpha}\vec{\sigma} \\ \alpha_0\mathbf{1} - i\vec{\alpha}\vec{\sigma} & \epsilon_b\mathbf{1} \end{pmatrix},$$

with $\epsilon_{a,b}$, α_0 and $\alpha_{x,y,z}$ real parameters. Show that the eigenvalues of this matrix are twofold degenerate, $E_\pm = (\epsilon_a+\epsilon_b)/2 \pm \Delta = (\epsilon_a+\epsilon_b)/2 \pm \sqrt{\alpha_0^2 + |\vec{\alpha}|^2 + (\epsilon_a-\epsilon_b)^2/4}$. (Hint: in spin space, use the eigenbasis of the operator $\vec{\alpha}\vec{\sigma}$.)

b. **(15pts)**

Now proceed as in the previous exercise. Construct the distance, $\mathrm{d}s^2 = \mathrm{Tr}(\mathrm{d}H\mathrm{d}H)$, from that the metric tensor, and show that the invariant measure is $\mathrm{d}\mu(H) = C\mathrm{d}\epsilon_a\mathrm{d}\epsilon_b\prod_k \mathrm{d}\alpha_k$. Express the full Gaussian unitary distribution, $\propto \mathrm{d}\mu(H)e^{-\lambda\mathrm{Tr}(H^2)}$ in terms of these six real parameters. Next, introduce spherical coordinates (Δ for the splitting, and θ_1, θ_2 θ_3 and ϕ for the α's and $(\epsilon_a-\epsilon_b)/2$). Compute the Jacobian, and reexpress the distribution in terms of these variables. Integrate over the angles, and obtain the distribution of Δ. Finally, determine the average level spacing, $\delta\epsilon \equiv 2\langle\Delta\rangle$, and derive the distribution of the dimensionless level spacing, $s \equiv 2\Delta/\delta\epsilon$.

2.1 (15pts+10pts) You can use Mathematica or MatLab for this exercise, or any other programming language. If you code in C or Pascal, you could consider using the numerical recipes routines for diagonalization.

Consider the following two dimensional Hamiltonian with periodic boundary conditions:

$$H = -\sum_{i=1}^{N}\sum_{j=1}^{N}(c_{i,j}^\dagger c_{i+1,j} + c_{i,j}^\dagger c_{i,j+1} + h.c.) + \sum_{i,j}\epsilon_{i,j}\; c_{i,j}^\dagger c_{i,j}\;,$$

where the $\epsilon_{i,j}$'s denote independent random variables in the interval $[-1,1]$.

a. **(8pts)** Diagonalize numerically the above Hamiltonian for various realizations of the disorder. [Construct operators $\Phi_E \equiv \sum_i \phi_i(E) c_i$ that satisfy $[H,\Phi_E] = -E\;\Phi_E]$. To have reasonable run times, use values $N \sim 30$.

b. **(7pts)** Do the statistics for the level spacings s for energies in the interval $E \in [-0.2, 0.2]$. (For a given realization of disorder, compute $s_i = E_{i+1} - E_i$ for $E_i \in [-0.2, 0.2]$ (allow E_{i+1} to be outside this interval, otherwise you introduce artificial cut-off errors). Do that for several realizations of the disorder, until you get good statistics. Be careful with the normalization of the numerically computed distribution function. For instance, if you use a mesh of spacing Δs to do the statistics, then you have $P(s \in [s_0 - \Delta s/2, s_0 + \Delta s/2]) \approx P(s_0)\;\Delta s$, with $P(s_0)$ the probability density you want to estimate at point s_0. Make sure that Δs is small enough (must be smaller than typical level spacing, $\delta\epsilon$!).

c. **(+10pts)** Determine the universal correlation function $C(s-s')$: $\langle \varrho(E)\varrho(E')\rangle = \langle\varrho(E)\rangle\langle\varrho(E')\rangle C((E-E')/\delta\epsilon))$.

2.2 (10pts) Consider free electrons ($m = \hbar = 1$) in a two-dimensional box of size $L_x = 1000$ and $L_y = 1000\;\pi$. Make a statistics of the level spacing for states with energy $1 < E < 1.1$. Measure energy separations in the average energy separation Δ, $s \equiv \Delta E/\Delta$. Estimate Δ analytically and compare it to your numerics. Discuss the distribution function $P(s)$.

[Hint: You will have to create a vector variable that will contain the energies of states with energies $1 < E < 1.1$. Then you have to order the energy of these states. You will have to create another array to make the statistics, where you just compute, how many states you have with separation s. Be careful, and properly normalize the distribution function $P(s)$. You can solve this problem in any programming language you like.]

3. (20pts) Weak localization correction for a cavity with time reversal symmetry
In this problem, we shall determine the weak localization correction to the average conductance of a cavity within the circular orthogonal ensemble (COE).

a. **(6pts)** First, analyze the structure of the S-matrix. Repeat the derivation at class to show that, in the presence of time reversal symmetry (and in the absence of spin), the S-matrix of a cavity is symmetrical, $S = S^T$. Show that any unitary matrix can be represented as $S = UDU^\dagger$, with U a unitary matrix, and D a diagonal matrix containing the eigenvalues of S, all on the unit circle, $s_\alpha = e^{i\phi_\alpha}$. Now prove that - with an appropriate phase choice - any symmetrical unitary matrix can be written as $\Omega^T\Omega$, with Ω a unitary matrix. Argue that $\Omega \in$ CUE.

b. **(2pts)** Now follow the derivation at class, and consider a cavity with N channels on the left and N channels on the right. Using the Landauer-Büttiker formula, $g = hG/e^2 = T = \sum_{i\in L}\sum_{j\in R}|S_{ij}|^2$, show that the expectation value of the transmission is given as

$$\langle T\rangle = 2N^3\, M, \quad \text{with } M = \langle|\Omega_{\alpha i}|^2|\Omega_{\alpha j}|^2\rangle_{i\neq j}.$$

c. **(12pts)** Determine M. Use the fact, that every column of Ω can be thought of as a real unit vector of dimension $d = 4N$, $x = \{\mathrm{Re}\Omega_{11}, \mathrm{Im}\Omega_{11}, \mathrm{Re}\Omega_{12}, \dots\} = \{x_1, x_2, \dots, x_{4N}\}$. Introduce the surface of the d-dimensional unit sphere as

$$A_d \equiv \int \mathrm{d}x_1 \dots \mathrm{d}x_d\, \delta(1 - (x_1^2 + \dots + x_d^2)).$$

Introduce furthermore the integrals, $I_n \equiv \int_0^\pi \mathrm{d}\theta \sin^n(\theta)$. Show that the following relations hold:

$$I_n = \frac{n-1}{n} I_{n-2}, \quad A_n = I_{n-2}A_{n-1}.$$

Using these relations evaluate $\langle|\Omega_{11}|^2\rangle$ and show that it is simply $1/2N$. Then, to evaluate M, first show that $M = \langle|\Omega_{11}|^2|\Omega_{12}|^2\rangle = 4\langle x_1^2 x_2^2\rangle$. Next show using the fact that x is a unit vector that

$$d\langle x_1^4\rangle + d(d-1)\langle x_1^2 x_2^2\rangle = 1.$$

Evaluate then $\langle x_1^4 \rangle$ and show that it is $\langle x_1^4 \rangle = 3/(d(d+2))$, from which one obtains

$$M = \frac{1}{2N(2N+1)}, \quad \text{and} \quad \langle T \rangle = \frac{N}{2}\frac{2N}{2N+1}.$$

This formula implies that, in the presence of time reversal symmetry, particles entering the chaotic cavity preferentially leave it towards the lead they came from. [Hint: evaluate for $d = 4N$

$$\langle x_1^2 \rangle = \frac{1}{A_d}\int \mathrm{d}x_1 \ldots \mathrm{d}x_d \, x_1^2 \, \delta(1 - (x_1^2 + \cdots + x_d^2))$$

by observing that the first term, $1 - x_1^2$, can be removed from the Dirac delta by appropriately rescaling $x_2, \ldots, x_d$, and then change variables, $x_1 \to \cos(\theta)$.]

II. NOISE AND NOISE SPECTRUM

4. (16pts) Noise of sequential tunneling through a single-level quantum dot
Consider a single-level quantum dot as described in Sections V/1, V/3, V/7 of Lecture 5 (*Noise in mesoscopic circuits*). Assume that a source-drain bias is applied, and current flows through the quantum dot via sequential tunneling. The temperature is zero.

a. **(8pts)** (50% of points) The tunnel rate from the source lead to the dot Γ_L is the same as the tunnel rate from the dot to the drain lead Γ_R, that is, $\Gamma_L = \Gamma_R = \Gamma$. Calculate the Fano factor using the cumulant generating function method as introduced on the lecture and in the lecture notes.

b. **(8pts)** Generalize for the result for unequal tunnel rates, $\Gamma_L = \eta\Gamma$, $\Gamma_R = \Gamma$.

5. (15pts) Quantum noise of a conductor acting on a nearby spin qubit
Consider a one-dimensional single-channel nanowire conductor with a mesoscopic scatterer limiting the transmission to $\tau = 0.1$. The conductor is voltage-biased by $V = 1$ mV, and the temperature is $T = 100$ mK. A nearby electron spin is Zeeman split by an external magnetic field of 1 Tesla pointing parallel to the wire. The spin qubit feels the quantum noise of the magnetic field created by the current flowing through the voltage-biased conductor. Assume that the spin's g-factor is 2.

a. **(5pts)** Calculate the effective temperature of the spin qubit.

b. **(2pts)** Estimate the coupling constant A between the wire current $\hat{J}$ and the spin $\hat{\sigma}_x$, if the spin is located at 10 nm distance from the wire. Express its value in picoelectronvolt-per-nanoampere. (The coupling constant A was defined in Lecture 6, Section V.)

c. **(8pts)** Calculate the relaxation time of the spin qubit. Plot the result in the bias-voltage range $0 < V < 1$ mV and temperature range $0 < T < 100$ mK, e.g., using a surface plot or a density plot.

Remark: In the published handwritten lecture notes of Lecture 7, Section VI/B, there is a typo in the prefactor of $S(\omega)$: the $\hbar$ should be corrected to h.

6. (20pts) Quantum noise of a three-terminal junction
Consider a junction of three quantum wires, where the wires (terminals) are labelled 1, 2, and 3. Each wire supports a single propagating channel, the scattering matrix of the junction is completely symmetric with respect to the permutations of the three terminals, and the reflection and transmission probabilities are all 1/3.

a. **(4pts)** Calculate the thermal current noise in lead 1 in equilibrium, as the function of temperature T and frequency ω.

b. **(16pts)** Consider the situation when lead 1 is voltage-biased with voltage V, while leads 2 and 3 are grounded. Calculate the average current and the current noise in all leads 1, 2 and 3.

Remark: Besides your own notes taken at the lecture, the review paper of Blanter and Buttiker (arXiv:cond-mat/9910158, sections II. C and II. D) can also be useful to reconstruct the derivation of the average current and the current noise.

III. TRANSPORT THROUGH QUANTUM DOTS

7.1 (20pts) Rate equation for a quantum dot (grain) with dense levels.
Repeat the derivation of the master equation discussed at class for the SET for the case where you consider the three possible states, $\hat{N} = -1, 0, 1$. Introduce the corresponding probabilities, P_0 and $P_\pm$. For the sake of simplicity assume that the SET is *completely symmetrical.* Denote the difference of the charging energies by $\Delta E_\pm \equiv E_\pm - E_0$.

a. **(10pts)** Construct the following steady state master equations:

$$\frac{dP_+}{dt} = P_0 W_{0\to+} - P_+ W_{+\to 0} \equiv 0 \,, \tag{1}$$

$$\frac{dP_0}{dt} = P_+ W_{+\to 0} + P_- W_{-\to 0} - P_0 W_{0\to+} - P_0 W_{0\to-} \equiv 0 \,, \tag{2}$$

$$\frac{dP_-}{dt} = P_0 W_{0\to-} - P_- W_{-\to 0} \equiv 0 \,. \tag{3}$$

Determine the rates W as we did at class (assuming a continuum of states, and a corresponding dimensionless conductance, $g_L = g_R = g$). Then determine the stationary values of $P_{0,\pm}$ from the above equations. [Note that at class we defined the transition probabilities slightly differently, and they contained the probabilities $P_{\pm,0}$.] Remember that the rates have two contributions, corresponding to tunneling processes from/to the right and left, and introduce accordingly $W^L_{\alpha\to\beta}$ and $W^R_{\alpha\to\beta}$. This is useful for the second part of this problem.

b. **(10pts)** Now compute and plot the current through the device as a function of bias voltage V for various values of the dimensionless gate voltage n_G. [Use that $E_N = E_C(N - n_G)^2$.] Plot the linear conductance as a function of n_g, and finally the differential conductance as a function of V for various values of n_G. Show that you indeed have a diamond structure as argued at class. Check the energies emerging in the differential conductance. [For these plots you can use $T = 0.1 E_C$, *e.g.*.]

7.2 (21+9pts) Rate equation for a quantum dot with a single level (simpler that 3.1 !).
Consider a quantum dot described by the Hamiltonian $H = H_{lead} + H_{dot} + H_t$:

$$H_{lead} = \sum_{\xi,\sigma} (\xi + \mu_L) L^\dagger_{\xi,\sigma} L_{\xi,\sigma} + \text{“}L \leftrightarrow R''\tag{4}$$

$$H_{dot} = \sum_\sigma E_+ \, |\sigma\rangle\langle\sigma| + E_0 |0\rangle\langle 0| \tag{5}$$

$$H_t \; = t_L \sum_{\xi,\sigma} (L^\dagger_{\xi,\sigma} |0\rangle\langle\sigma| + h.c.) + \text{“}L \leftrightarrow R''. \tag{6}$$

Here $|\sigma\rangle$ and $|0\rangle$ denote the dot states with one electron of spin σ and no electrons, respectively. Note that we assumed a large level spapcing in this case, so this is just the opposite of the limit we considered at class ! Now repeat the derivation of the master equation for this system.

a. **(7pts)** Show that the rate of an electron jumping into the dot from the left is given by

$$W_{0\to+} = 2\Gamma_L \; f(\Delta E - \mu_L) \, P_0$$

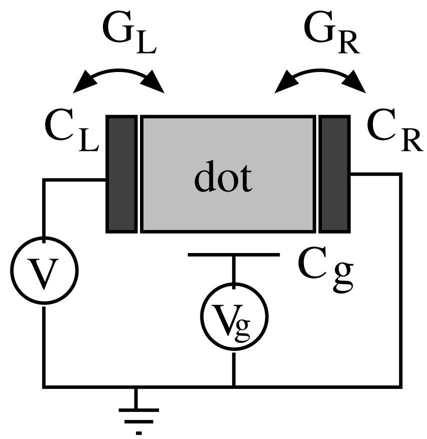
in the Born approximation, with $\Gamma_L = 2\pi\varrho_0 t_L^2$ the width of the level, $\Delta E = E_+ - E_0$, f the Fermi function, and P_0 the probability that the dot has no electron. Note the prefactor in front, that is due to the spin! Write down the equations for all other electron transfer processes.

b. **(7pts)** Construct the master equation for the probabilities P_0 and P_+ of having no or one electron on the dot. Determine the stacionary solution and express the current from these equations.

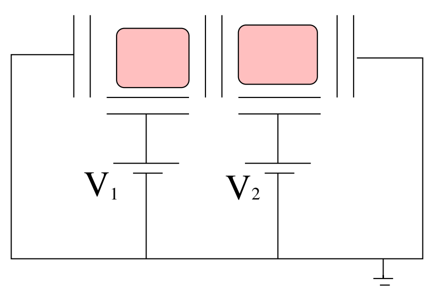
c. **(7pts)** Now determine the linear conductance of the dot as a function of temperature and ΔE, show that the Coulomb blockade peak is asymmetrically shifted. What is it's height? Discuss the problem with the peak height's temperature dependence! What do you think the solution is?

d. **(+9pts)** Optional: Generalize the calculation for the case where the energies of the spin up and spin down dot states are split by a magnetic field, $E_\uparrow - E_\downarrow = B$. Compute the polarization of the current. Show that the current is spin polarized if $B > T$.

8.1 (10pts) Compute the energy of a single electron transistor shown in the figure as a function of gate and bias voltages, and for a fixed number n of electrons on the island. [Hint: Assume first that no charge has been transferred through the capacitor C_R, and that tunneling only occurred through C_L. Then discuss what happens if some electrons DO tunnel through this capacitor.]



8.2 (15pts)
Consider two identical unbiased SET's in series. (See figure.) Assume that all capacitors are the same.



a. **(5pts)** Derive the energy of the circuit for fixed number of particles n_1 and n_2 on the two dots.

b. **(5pts)** Make a plot on the V_1, V_2 plane, and draw the regions of the various minimum energy states (indicate in every regime the optimum values of n_1 and n_2.

c. **(5pts)** Can you make a turnstyle of the double dot system in series, i.e. a transistor where you transfer charge from one side to the other by applying an AC modulation on n_{g1} and n_{g2} in every cycle, so that the current is just $I = e\omega$?

IV. SUPERCONDUCTING GRAINS

9 (15pts) Phase description of a superconducting grain

Consider a superconducting Island attached to a superconducting lead, as described by the Hamiltonian,

$$H = \frac{1}{2} E_C \, (\hat{n} - n_g)^2 - \frac{1}{2} E_J \sum_n (|n+1\rangle\langle n| + \text{h.c.}) \ . \tag{7}$$

a. **(2pts)** As a warm-up, reproduce the analysis at class: introduce the states $|\phi\rangle \equiv \sum_n e^{-i\phi\, n}|n\rangle$, and show that in the phase representation, $|f\rangle \equiv \int_{-\pi}^{\pi} \frac{d\phi}{2\pi} f(\phi)|\phi\rangle$, $\hat{n}|f(\phi)\rangle = | - i\partial_\phi f(\phi)\rangle$. Also, act with the shift operator

$\sum_n |n+1\rangle\langle n|$ on a state $|f(\phi)\rangle$ and show that it is just $e^{i\hat{\phi}}$. Rewrite the Hamiltonian in phase representation, and show that it reads

$$H = -\frac{1}{2} E_C \,(\partial_\phi - i\, n_g)^2 - E_J \cos(\phi) \tag{8}$$

b. **(3pts)** Equation of motion:
Show for $n_g = 0$ that the operators $\hat{\phi}$ and $\hat{n}$ satisfy the classical equations of motion of a quantum pendulum in the Heisenberg picture. [You can use just the commutation relations or the phase representation of the Hamiltonian.] Linearize these equations in the limit of small ϕ (a good approximation for large Josephson energy) , and show that the oscillation frequency is $\omega = \sqrt{E_J E_C}$, which we called the plasmon frequency. Discuss the general dynamics of the classical solution.

c. **(5pts)** Now solve the quantum problem in the basis of $\hat{n}$. For simplicity, consider only states with $|n| < 30$, and plot the first few eigenenergies of Eq.(7) as a function of the dimensionless gate voltage n_g for $E_J/E_C = 0.2$, $E_J/E_C = 1$, and $E_J/E_C = 5$. (You shoud obtain a periodic function.)

d. **(5pts)** What are the eigenfunctions of $\hat{n}$, i.e. $\langle\phi|n\rangle$? Construct now the ground state eigenfunction $f_0(\phi)$ and the eigenfunction $f_1(\phi)$ of the first excited state of the superconducting grain in ϕ-space for $n_g = 0$ and $E_J/E_C = 0.2$, 1, and 5, and plot the phase distribution, $|f_{0,1}(\phi)|^2$. Do this also at the charge transition point, $n_g = 1/2$!

10. (15pts) Soft boson solution of Richardson problem
Details will follow.