Final exam – Friday January 12th 2024 (9AM-12PM) Topic: density fluctuations in 1D electron gases

Some advice and guidelines:

- You can use handwritten notes from the lectures and the tutorials, but no book, computer, or phone
- Write your name and page number on each page, and indicate the total number of pages on page 1
- Address first the questions that you feel confident about
- All questions (and sub-questions) are independent of each other, do not get stuck
- Avoid giving too lengthy answers
- Write clearly and highlight the important results, only a correct argumentation will give full points
- Some hints are given as underlined text (use them!)
- The exam is probably too long, don't worry about it!
- $\hbar = 1$ is set throughout

1 General questions

Your answers to these questions do not require any detailed calculations. These questions are fully independent from the main exam problem.

1. Here are a few many-body wavefunctions for particles in \mathbb{R}^3 , without spin:

(a)
$$\Psi_1(\vec{r_1}, \vec{r_2}) = e^{-|\vec{r_1} - \vec{r_2}|}$$

- (b) $\Psi_2(\vec{r}_1, \vec{r}_2) = \sinh[(\vec{r}_1 \vec{r}_2).\vec{e}_z]$
- (c) $\Psi_3(\vec{r}_1, \vec{r}_2, \vec{r}_3) = \cos[\vec{r}_1 . (\vec{r}_2 \times \vec{r}_3)] e^{-|\vec{r}_1|^2 |\vec{r}_2|^2 |\vec{r}_3|^2}$

Indicate for each if it is symmetric or antisymmetric, and argue if it is square integrable.

2. Consider a set of one-body wavefunctions $\Phi_{\mu}(\vec{r})$, with $\mu = 1, 2, 3, 4$ only (no spin). Using second quantization notation for fermionic many-body states $|n_1, n_2, n_3, n_4\rangle = (c_1^{\dagger})^{n_1} (c_2^{\dagger})^{n_2} (c_3^{\dagger})^{n_3} (c_4^{\dagger})^{n_4} |0\rangle$, where $n_{\mu} = 0, 1$ is the occupation of orbital μ , enumerate a complete basis of antisymmetric states for N = 1 particles, then for N = 2particles. Can one construct a non-trivial Fock space for N = 10 particles with those states?

3. Give three different types of symmetry-breaking phases found in electronic systems at low temperatures, and write the corresponding order parameter as a bilinear form with fermionic creation/annihilation operators.

4. Let's imagine putting a nanometer-sized conducting tip above a 2D electron gas. Putting the tip at a finite electrical potential, which observable \hat{B} of the gas is perturbed? Which other observable \hat{A} do you imagine could be measured in such a setup? If the tip is moved laterally, on which spatial length scales would you expect to see some variations of the measured observable, assuming the gas contains some impurities?

2 Density fluctuations in good metals

We will stick for simplicity to 1D fermions in all what follows. Our main goal is to investigate how density fluctuations in an electron gas evolve from weak to strong interactions, and to learn how they give information about the possible underlying electronic states: Fermi liquid, Luttinger liquid, or Wigner crystal.

1. We will start with non-interacting fermions, assumed to be spinless for simplicity. The 1D dispersion relation is taken as linear: $\epsilon_k = v_F |k|$, with v_F the Fermi velocity. Fixing a positive chemical potential $\mu > 0$, sketch graphically the filling of the Fermi sea and identify the Fermi wavevector k_F on this plot. Write the energy dispersion E(k,q) for a particle-hole excitation with a particle of momentum k + q and a hole with momentum k. <u>Hint:</u> beware, there are two possible electronic branches. Sketch the resulting particle-hole continuum, and identify a collective mode. Can you comment on the difference for the collective mode with respect to the case of quadratic dispersion seen in the exercises?

2. From the density operator $\hat{n}(x) = \Psi^{\dagger}(x)\Psi(x) = \int \frac{dk}{2\pi} \int \frac{dk'}{2\pi} e^{i(k-k')x} c_k^{\dagger} c_{k'}$, show that the average density is uniform in the ground state (filled Fermi sea) and reads $\langle \hat{n}(x) \rangle = k_{\rm F}/\pi \equiv n_0$.

3. Compute the density-density correlation function $g(x) = \langle \hat{n}(x)\hat{n}(0) \rangle$ in the ground state using Wick's theorem. Perform the k-integral and show that:

$$g(x) = n_0^2 - \frac{\sin^2(k_F x)}{\pi^2 x^2} = n_0^2 - \frac{1}{2\pi^2 x^2} + \frac{\cos(2k_F x)}{2\pi^2 x^2}.$$
 (1)

We observe that both the slow amplitude term and the Friedel-like $2k_{\rm F}$ fast oscillating term both decay as $1/x^2$ at long distances. This is a hallmark of Fermi-liquid states in 1D. Compute g(0) and argue about its value. Compute g(x) at $x = \infty$ and also explain its value.

4. We now introduce electron-electron interactions (still for spinless fermions):

$$\hat{H} = \sum_{k} \epsilon_{k} c_{k}^{\dagger} c_{k} + \frac{1}{2\mathcal{V}} \sum_{k,k',q} V_{q} c_{k+q}^{\dagger} c_{k'-q}^{\dagger} c_{k'} c_{k}, \qquad (2)$$

with \mathcal{V} the spatial volume. Assuming translation invariance, write explicitly the Hartree-Fock many-body wavefunction in second quantized form. Show that the quasiparticle energies are given by the following expression $E_k = \epsilon_k + (1/\mathcal{V}) \sum_{k'} \theta(k_{\rm F}^* - |k'|) (V_0 - V_{k'-k})$, with $\theta(k)$ the Heaviside function, and $k_{\rm F}^*$ the renormalized Fermi wavevector (it could naively be affected by interactions). Fixing the electron density to n_0 , and assuming the renormalized dispersion relation E_k to be monotonous, show that in fact $k_{\rm F}^* = k_{\rm F}$ (this is a peculiar case of the Luttinger theorem). What does that imply for the density-density correlation function g(x)? Going beyond the Hartree-Fock calculation (do not attempt it of course), and assuming a Fermi liquid state is obtained, what could you say about the behavior of the slow amplitude term and of the $2k_{\rm F}$ term in g(x) at long distances?

3 Strong interaction limit: from Wigner crystal to Luttinger liquid

1. In this second part, we consider the opposite limit of very strong Coulomb interactions (relative to the kinetic energy), which leads classically to a crystalline state where electrons are localized at position $x_i^0 = ai$, with $a = 1/n_0$ the inter-electron distance and n_0 the average density. Fluctuations around the equilibrium position will be described by collective phonon-like variables $\hat{\phi}_i$, so that the electron position operator (in first quantization) is $\hat{x}_i = ai + a\hat{\phi}_i/\pi$ and the electron momentum operator $\hat{p}_i = \pi \hat{\Pi}_i$ (the π factors are just a rescaling). In the continuum limit $a \to 0$, with x = ai kept finite, show that the previous operators behave as conjugate fields at the quantum level, namely $[\hat{\phi}(x), \hat{\Pi}(x')] = i\delta(x - x')$. Express also the kinetic energy of the electron gas as:

$$\hat{H}_0 = \int dx \frac{\pi^2}{2ma} [\hat{\Pi}(x)]^2,$$
(3)

with m the electron mass.

2. Show that the electron density operator simplifies in the continuum limit to the form $\hat{n}(x) \simeq n_0 - \partial_x \hat{\phi}(x)/\pi$. <u>Hint:</u> argue physically what happens when one of the phase differences $\hat{\phi}_{i+1} - \hat{\phi}_i$ winds by $-\pi$.

Assuming for simplicity short-range Coulomb interaction with amplitude V_0 (although this is not realistic), express the interaction part of the energy (substracting the classical neutralizing background) as:

$$\hat{H}_{1} = \int \mathrm{d}x \frac{V_{0}}{2\pi^{2}} [\partial_{x} \hat{\phi}(x)]^{2}.$$
(4)

We reparametrize the full Hamiltonian as:

$$\hat{H} = \hat{H}_0 + \hat{H}_1 = \frac{1}{2\pi} \int dx \Big\{ v K \pi^2 [\hat{\Pi}(x)]^2 + \frac{v}{K} [\partial_x \hat{\phi}(x)]^2 \Big\},\tag{5}$$

with v the renormalized Fermi velocity and K a dimensionless interaction parameter. Extract v and K as a function of the microscopic parameters in $\hat{H}_0 + \hat{H}_1$ and prove that $v = v_F/K$, with v_F the bare Fermi velocity. <u>Hint:</u> show that $a = \pi/(mv_F)$. Argue why $K \ll 1$ describes the regime of weak kinetic energy respective to the strong Coulomb energy. Why is the bosonic Hamiltonian \hat{H} much simpler than its original formulation in terms of interacting fermions?

3. It will be useful to compute the retarded (bosonic) correlation function of the collective mode:

$$G^{\mathrm{R}}_{\phi}(x,t) = -i\theta(t) \langle [\hat{\phi}(x,t), \hat{\phi}(0,0)] \rangle, \tag{6}$$

with $\hat{\phi}(x,t) = e^{i\hat{H}t}\hat{\phi}(x)e^{-i\hat{H}t}$. For all x, why is this function continuous at t = 0? Taking a first derivative, show that:

$$\partial_t G^{\mathbf{R}}_{\phi}(x,t) = -i\theta(t)\pi K v \langle [\hat{\Pi}(x,t), \hat{\phi}(0,0)] \rangle.$$
⁽⁷⁾

<u>Hint</u>: you will need to compute the commutator $[\hat{H}, \hat{\phi}(x)]$ using the fields commutation relations. Taking a second derivative, show similarly that:

$$\partial_{tt} G^{\mathrm{R}}_{\phi}(x,t) = -\pi v K \delta(t) \delta(x) + v^2 \partial_{xx} G^{\mathrm{R}}_{\phi}(x,t).$$
(8)

Going to Fourier space both in frequency and momentum, obtain the bosonic propagator:

$$G_{\phi}^{\rm R}(k,\omega) = \frac{\pi K v}{-v^2 k^2 + (\omega + i0^+)^2}.$$
(9)

4. Using the bosonic language, we are now equipped to compute the wanted density-density correlation function $g(x) = \langle \hat{n}(x)\hat{n}(0) \rangle$, using that $\hat{n}(x) \simeq n_0 - \partial_x \hat{\phi}(x)/\pi$ for slowly varying charge fluctuations. You can start with $g(x) = n_0^2 - (1/\pi^2)\partial_{xx}\langle \hat{\phi}(x)\hat{\phi}(0) \rangle$ (justify the negative sign). Use the fluctuation-dissipation theorem at zero temperature to relate the unsymmetrized correlation function $S_{\phi}(x,t) = \langle \hat{\phi}(x,t)\hat{\phi}(0,t) \rangle$ to the retarded propagator (6) taken in frequency domain. Using that $g(x) = n_0^2 - (1/\pi^2)\partial_{xx}\int d\omega S_{\phi}(x,\omega)$, you should obtain:

$$g(x) = n_0^2 + \frac{1}{\pi^2} \int_{-\infty}^{+\infty} \frac{\mathrm{d}k}{2\pi} k^2 e^{ikx} \int_0^{+\infty} \frac{\mathrm{d}\omega}{\pi} \mathrm{Im} G_{\phi}^{\mathrm{R}}(k,\omega).$$
(10)

Inserting formula (9), and performing the ω -integral, derive the expression $g(x) = n_0^2 + \frac{K}{4\pi^2} \int_{-\infty}^{+\infty} dk |k| e^{ikx}$. One sees that this integral is ultra-violet divergent, but you can regularize it phenomenologically with a cutoff term $e^{-|k|/k_{\rm F}}$. At long distances $|k_{\rm F}x| \gg 1$, you should find $g(x) \simeq n_0^2 - K/(2\pi^2 x^2)$. The amplitude of the slow envelope in g(x) is thus renormalized by interactions. Comparing to the exact result (1), we thus extract the dimensionless interaction parameter K = 1 for free fermions.

5. We finally investigate the $2k_{\rm F}$ oscillations in the density-density correlation function using the bosonic language, generalizing the $\cos(2k_{\rm F}x)$ term of g(x) in Eq. (1) to the non-trivial case of interacting fermions in 1D. Argue physically why the oscillating contribution to the electron density behaves like $\hat{n}_{2k_{\rm F}}(x) \propto e^{i2k_{\rm F}x}e^{2i\hat{\phi}(x)}$ +h.c. (up to a prefactor). We will employ the following general result (do not prove it, but it follows readily from the Baker-Campbell-Hausdorff formula) that $\langle e^{\hat{O}} \rangle = e^{\langle \hat{O}^2 \rangle/2}$, with \hat{O} a linear bosonic operator, and the average being taken in the ground state of a quadratic Hamiltonian. Show from this result that the $2k_{\rm F}$ term in g(x) scales as $\left[e^{-2\langle [\hat{\phi}(x)+\hat{\phi}(0)]^2 \rangle} + e^{-2\langle [\hat{\phi}(x)-\hat{\phi}(0)]^2 \rangle}\right] \cos(2k_{\rm F}x)$. Using the equal-time unsymmetrized correlator $\langle \hat{\phi}(x)\hat{\phi}(0) \rangle$ already computed previously, deduce that $\langle [\hat{\phi}(x)\pm\hat{\phi}(0)]^2 \rangle = (K/2)\int dk e^{-|k|/k_{\rm F}}(1\pm e^{ikx})/|k|$. For $x \to \infty$, show the asymptotic behavior: $\langle [\hat{\phi}(x)-\hat{\phi}(0)]^2 \rangle \propto K \log |k_{\rm F}x|$. Note that the correlator $\langle [\hat{\phi}(x)+\hat{\phi}(0)]^2 \rangle$ is infra-red divergent for all x, so that the associated exponential term $e^{-2\langle [\hat{\phi}(x)+\hat{\phi}(0)]^2 \rangle}$ cancels out in g(x). The final result is thus that g(x) contains an oscillatory term $\cos(2k_{\rm F}x)e^{-2K\log |k_{\rm F}x|} = \cos(2k_{\rm F}x)/|k_{\rm F}x|^{2K}$ displaying an anomalous power law decay, which is prototypical of Luttinger liquids (*i.e.* 1D non-Fermi liquids). How do you recover the non-interacting limit? In the opposite limit of infinitely large interaction $(K \to 0)$, check that a Wigner crystal forms. Physically, why is there no crystalline order for large but finite ($0 < K \ll 1$) interaction?