Problem set 2 for the course "Many -body physics 2", 2018

Rules: You can solve any number of problems. You can collect 30 points at maximum, and you must collect 10 points to pass. You can help each-other and discuss, give hints to each-other (this is even encouraged), but you are not allowed to copy.
Deadline: May 22.

1. (10 p) Investigation of the polarization bubble.

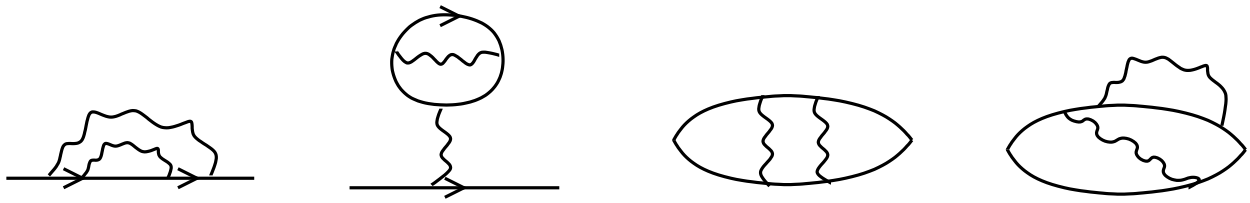
a. **(1 p)** Use the momentum space diagrammatic rules, and construct the integral expression of the polarization bubble $\Pi_0(\omega, \mathbf{q})$ (i.e., the unperturbed density-density time-ordered correlation function) of a 3-dimensional electron gas.

b. **(3 p)** Evaluate first the frequency integral using the tricks shown at class, do the analytical continuation, and derive the expression for the retarded density-density response function:

$$\chi_0(\omega, \mathbf{q}) = -2 \int \frac{d^3\mathbf{p}}{(2\pi)^3} \frac{f(\mathbf{p}) - f(\mathbf{p}+\mathbf{q})}{\omega + \xi(\mathbf{p}) - \xi(\mathbf{p}+\mathbf{q}) + i\,\delta} \ .$$

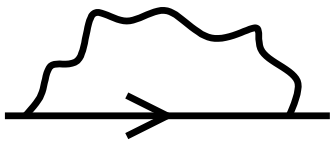
c. **(6 p)** Evaluate the imaginary part of χ_0, and plot it as a function of ω for various values of $q < 2p_F$ and for $q > 2p_F$, too. [Hint: Assume a parabolic dispersion, $\xi = (p^2 - p_F^2)/2m$, and introduce appropriate polar coordinates.] Remember that $\Im\chi(\omega, \mathbf{q})$ is proportional to the inelastic scattering cross section with energy transfer ω and momentum transfer $\mathbf{q}$.

2. (4 p) Application of diagram rules.
Write explicitly the self-energy- and density-density correlation function corrections both in real and in momentum space for the following diagrams: Watch out for the direction of arrows (not indicated), loops etc.. Only perfect



answers give you points (no sign or momentum conservation mistakes etc.).
3. (10 p) Evaluation of the Fock term for an interacting electron gas.

a. **(1 p)** Using the diagrammatic rules, write down the momentum space expression for the "Fock term", corresponding to the diagram shown below. (In reality, the Fock term contains the full Green's function, but for an interacting electron gas it turns out to be the same as the diagram below.)



Evaluate first the frequency integral and obtain the following expression:

$$\delta\Sigma_F(\mathbf{p}) = -\int_{|\mathbf{q}|<\mathbf{p_F}} \frac{d^3\mathbf{q}}{(2\pi)^3} \frac{4\pi\ e^2}{|\mathbf{p}-\mathbf{q}|^{\mathbf{2}}} \ .$$

Be careful with closing the contour.

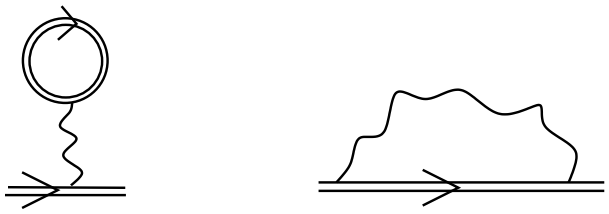
a. **(4 p)** Evaluate the previous integral using polar coordinates to get the expression discussed at class.

b. **(5 p)** Evaluate the integral above using a Thomas-Fermi screened Coulomb interaction, too,

$$\frac{4\pi\ e^2}{|\mathbf{q}|^2} \to \frac{4\pi\ e^2}{|\mathbf{q}|^2 + q_T^2}\ .$$

Compute the renormalized Fermi velocity and show that it is finite at the Fermi energy. (You can also use Mathematica or Maple to carry out the integrals.)

4. (30 p) Atomic Hartree-Fock approximation. In this exercise you will show that the self-consistent diagrammatic approach discussed at class reduces to the usual Hartree-Fock approximation.



a. **(5 p)** First consider a non-interacting Hamiltonian of the form:

$$H = \int \mathbf{dr}\ \psi_\sigma^\dagger(\mathbf{r})\mathcal{H}(\mathbf{r})\psi_\sigma(\mathbf{r})\ . \tag{1}$$

Express the Green's function in terms of the eigenfunctions $\varphi_n(\mathbf{r})$ and eigenenergies ϵ_n of $\mathcal{H}(\mathbf{r})$ and show that it is given by

$$G(\mathbf{r}\sigma, \mathbf{r}'\sigma', \omega) = \sum_n \frac{\varphi_n(\mathbf{r}, \sigma)\varphi_n^\star(\mathbf{r}', \sigma')}{\omega - \epsilon_n + i\ \delta\ \mathrm{sgn}(\omega - \mu)}\ , \tag{2}$$

where we now explicitly displayed the dependence on the chemical potential, which we now defined as the energy of the last occupied state, and the label n incorporates the spin of the electrons. Express also $G^{-1}(\mathbf{r}\sigma, \mathbf{r}'\sigma', \omega)$ in a similar way. (Hint: Use the eigenstates $\varphi_n(\mathbf{r})$ to express the field operators, and then obtain first $G(\mathbf{r}\sigma, \mathbf{r}'\sigma', t)$ and from that $G(\mathbf{r}\sigma, \mathbf{r}'\sigma', \omega)$. To get $G^{-1}(\mathbf{r}\sigma, \mathbf{r}'\sigma', \omega)$, think of $G(\mathbf{r}\sigma, \mathbf{r}'\sigma', \omega)$ as an integral kernel, and use $G^{-1}(\omega) * G(\omega) = \delta(\mathbf{r} - \mathbf{r}')\delta_{\sigma\sigma'}$.)

b. **(5 p)** To obtain the Hatree-Fock equations, we shall assume that with some (yet undetermined) functions, $\varphi_n(\mathbf{r})$, the full Green's function takes on the form, (2), while the self-energy is just given by the Hartee term (or Hartree + Fock terms), shown in the figure.

As a first step, divide the atomic Hamiltonian into two parts, $H = H_0 + H_{\mathrm{int}}$:

$$H_0 = \sum_\sigma \int \mathbf{dr}\ \psi_\sigma^\dagger(\mathbf{r})[-\frac{1}{2M}\Delta_{\mathbf{r}} + V(\mathbf{r})]\psi_\sigma(\mathbf{r}) \tag{3}$$

$$H_{\mathrm{int}} = \frac{1}{2}\sum_{\sigma,\sigma'} \int \mathbf{dr}\ \int \mathbf{dr}' \frac{e^2}{|\mathbf{r} - \mathbf{r}'|^2}\psi_\sigma^\dagger(\mathbf{r})\psi_{\sigma'}^\dagger(\mathbf{r}')\psi_{\sigma'}(\mathbf{r}')\psi_\sigma(\mathbf{r})\ . \tag{4}$$

Evaluate first the Hartree diagram using the Ansatz (2) for the total Green's function, and show that the Hartree self-energy is

$$\Sigma^H(\mathbf{r}, \mathbf{r}', \omega) = \delta(\mathbf{r} - \mathbf{r}')\ \sum_{\epsilon_n < \mu} \int \mathbf{dr}'' \frac{e^2}{|\mathbf{r} - \mathbf{r}''|^2}\ |\varphi_n(\mathbf{r}'')|^2\ . \tag{5}$$

(Notice that in real space the self-energy is also an integral operator, and the multiplication in momentum space becomes a "convolution".)

c. **(5 p)** Prove that the inverse of the unperturbed Green's function, G_0^{-1}, can be expressed as

$$G_0^{-1}(\mathbf{r}, \mathbf{r}', \omega) = (\omega - \mathcal{H}^0(\mathbf{r}))\ \delta(\mathbf{r} - \mathbf{r}')\ , \tag{6}$$

with $\mathcal{H}^0(\mathbf{r}) = -\frac{1}{2M}\Delta_{\mathbf{r}} + V(\mathbf{r})$. [Hint: Show that $G_0^{-1} * G_0 = \delta(\mathbf{r} - \mathbf{r}')$.]

d. **(5 p)** Now consider the Dyson equation (written for G^{-1} as $G^{-1} = G_0^{-1} - \Sigma_H$) and show using the above expression that the self-consistent solution of the Dyson equation with the Hartree self-energy can be found in a form (2) provided that the φ_n's satisfy the following integral equation:

$$(-\frac{1}{2M}\Delta_{\mathbf{r}} + V(\mathbf{r}) + V^H(\mathbf{r}))\varphi_n = \epsilon_n\, \varphi_n \ , \tag{7}$$

$$V^H(\mathbf{r}) = \sum_{\epsilon_n<\mu} \int \mathbf{dr}'' \frac{e^2}{|\mathbf{r}-\mathbf{r}'|^2}\, |\varphi_n(\mathbf{r}'')|^2 \ . \tag{8}$$

[Hint: Act with the inverse G^{-1} as computed from Eq. (2) on the one hand, and also with $G_0^{-1} - \Sigma_H$ on the other hand, on φ_n.]

d. **(10 p)** Generalize the above procedure for the Fock diagram, too, and obtain the Hartree-Fock equations.

5. (25 p) Spin-spin correlation function and susceptibility for local electron-electron interaction.

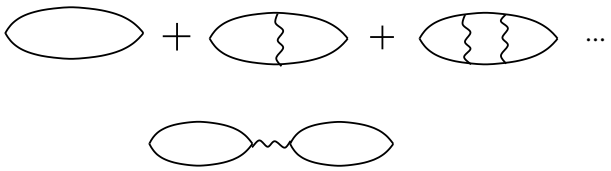
a. **(5 p)** First, compute the Fourier transform of the spin-spin correlation function of a non-interacting electron gas,

$$G_{\sigma\sigma} \equiv -i\langle T\{\sigma^z(\mathbf{r},t)\sigma^z(\mathbf{r}',t')\}\rangle_0 \ , \tag{9}$$

where $\sigma^i(\mathbf{r},t) = \sum_{\alpha\beta} \psi^\dagger_\alpha(\mathbf{r},t)\sigma^i_{\alpha\beta}\psi_\beta(\mathbf{r},t)$.

b. **(5 p)** Next show that the leading Coulomb diagrams discussed at class give no correction to the spin-spin correlation function. (Evaluate the simplest RPA-type diagram shown in the second line below, and show that the various terms cancel.)

c. **(10 p)** Now approximate the electron-electron interaction by a local interaction (this mimics a screened interaction, discussed at class), $V(x-x') = V_0\delta^4(x-x')$, and sum up in momentum space the "ladder" series shown in the Figure below. (These are the leading diagrams for the spin-spin correlation function.)



d. **(5 p)** Compute the renormalized spin susceptibility and recover the Pauli susceptibility for $V_0 = 0$. Is it increased or decreased by a repulsive electron-electron interaction? Try to explain it. What happens if you increase V_0?