Condensed Matter Physics II. – A.A. 2020-2021, May 07 2021

(time 3 hours)

Solve the following two exercises, each has a maximum score of 18 for a total of 36. A score between 33 e 36 corresponds to 30 cum laude, between 30 e 32 is renormalized to 30 (the maximum official score, without laude).

NOTE:

- Give all details which help in understanding the proposed solution. Answers which only contain the final result or not enough detail will be judged insufficient and discarded;
- If you are requested to give evaluation/estimates, do so using 3 significant figures.

Exercise 1: *Hartree -Fock in 1D for Fermions interacting with a short range repulsion, spin unpolarized*

Consider N spin 1/2 Fermions moving on the segment L with Hamiltonian

$$H = \sum_i^N \left[-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + v_b(x_i) \right] + \sum_{i<j} v(x_i - x_j) + U_{bb}; \tag{1}$$

$v(x) = v_0 \exp(-q_0|x|)$ with $v_0, q_0 > 0$, $v_b(x) = -\int dx' \rho_b\, v(x-x')$ is the interaction with an appropriate background with self-energy $U_{bb} = (1/2)\int dx \int dx' \rho_b^2\, v(x-x')$ and $\rho_b = N/L$. In the following we shall take PBC and when appropriate invoke the thermodynamic limit and restrict to spin unpolarized states, i.e., $N_\uparrow = N_\downarrow$.

5p 1. Demonstrate that a single determinant of plane waves is a HF solution for a generic $v(x)$.

2p 2. The demonstration above should involve the Fourier transform of $v(x)$, which we denote with $\tilde{v}(k)$ and should provide an expression for the HF eigenvalue $\varepsilon_{HF}(k)$ and for its exchange part, which we call $\varepsilon_x(k)$

2p 3. Specialize now to the pair potential given above and calculate $\tilde{v}(k)$. You should get quite easily an elementary function.

2p 4. Having $\tilde{v}(k)$ for the potential of interest, calculate explicitely now the exchange part of the HF eigenvalue $\varepsilon_x(k)$.

2p 5. Knowing $\varepsilon_{HF}(k)$, expand it around $k = 0$, to quadratic terms included.

2p 6. Provide and expression for the effective mass resulting from the above expansion.

Exercise 2: LD and linear response

Consider a non interacting electron un gas in 1 dimension. The static linear response function at $T = 0$ is define to be (in q space)

$$\chi_0(q) = -\frac{2}{L}\sum_k \theta(k_F - |k|)\left[\frac{1}{\varepsilon(k+q)-\varepsilon(k)} + \frac{1}{\varepsilon(k-q)-\varepsilon(k)}\right],$$

with $\varepsilon(k) = \hbar^2 k^2/2m$ the energy levels of the non interacting electrons.

1. Calculate $\chi_0(q)$, giving all relevant details of the calculation.
2. Sketch $\chi_0(q)$ as function of $Q = q/k_F$, for $Q \geq 0$. Comment on the behavior of $\chi_0(q)$ for $q < 0$ without drawing any figure.
3. Calculate the kinetic energy per particle $t(n)$ of the homogeneous electron gas in 1D, where n is the density and from it obtain $T^{LDA}[n]$, the kinetic energy functional in the local density approximation.
4. Consider now the electron gas under the action of an external potential $v(x)$, so that the total energy becomes $E[n] = T^{LDA}[n] + \int dx\, n(x)\, v(x)$, and write the extremum condition obeyed by the functional for given external potential, solving for $n(x)$. Beware that the variation must be taken with the constraint $\int dx n(x) = N$.
5. For $v(x) = 0$ the density is homogeneous, $n(x) = n$. Using the definition of response function in an homogeneous fluid,

   $$\chi(x-y) = \left[\frac{\delta n(x)}{\delta v(y)}\right]_{v=0},$$

   calculate the response function in LDA and take its Fourier transform:$\chi_{LDA}(q) = \int_{-\infty}^{\infty} dz\, \chi_{LDA}(x)\, e^{iqx}$.
6. In the expression found above eliminate the lagrange multiplier (i.e., the chemical potential) in favor of the homogeneous density n, compare the previous result with that of point 1, on the graph of point 2, and comment on the relation between the LDA and the exact result.