Estado Sólido I
Tarea 4: Modelo del Gas de Electrones Libres

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Nombre del Estudiante: _____

Problema 1   *Cohesive energy of the free electron Fermi gas*

We define the dimensionless lenght r_s as r_0/a_H, where r_0 is the radius of a sphere that contains one electron, and a_H is the Bohr radius $\hbar^2/e^2m$.

(a) Show that the average kinetic energy per electron in a free electron Fermi gas at 0 K is $2.21/r_s^2$, where the energy is expressed in rydbergs with $1 \text{ Ry} = me^4/2\hbar^2$.

(b) Show that the coulomb energy of a point positive charge e interacting with the uniform electron distribution of one electron in the volume of a sphere of radius r_0 (given by $\rho = -e/V$) is $-3e^2/2r_0$ or $-3/r_s$ in rydbergs. You can consider the point particle located at the origin of the sphere, and use the following expresion for the interaction:

$$V_C^+ = \int \frac{e\rho}{|\mathbf{r}|} d\mathbf{r}.$$

(c) Show that the coulomb self-energy of the electron distribution of the sphere is $3e^2/5r_0$ or $6/5r_s$ in rydbergs, using the following expression:

$$V_C^{self} = \int \frac{q(\mathbf{r})\rho}{|\mathbf{r}|} d\mathbf{r},$$

where $q(\mathbf{r})$ is the charge of the electron distribution at a given $\mathbf{r}$.

(d) Construct the total energy of the system, by summing the kinetic and both coulomb potential energies. Show that the equilibrium value for r_s is 2.46, and find the cohesive energy value (the minimum of energy).

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Problema 2   *Chemical potential in 1D and 2D*

Show that the chemical potential of a Fermi gas in $1D$ and $2D$ are given by:

$$1D: \quad \mu(T) = \epsilon_F \left[1 + \frac{\pi^2}{12} \left(\frac{k_B T}{\epsilon_F} \right)^2 \right] \quad \forall \ \epsilon_F = \frac{\hbar^2 \pi^2}{2m} n^2,$$

$$2D: \quad \mu(T) = k_B T \ln \left[\exp \left(\frac{\pi n \hbar^2}{m k_B T} \right) - 1 \right],$$

for n electrons per unit length or area.

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Problema 3   *Kinetic energy, pressure, and bulk modulus of an electron gas*

(a) Show that the kinetic energy of a three-dimensional gas of N free electrons at 0 K is

$$U_0 = \frac{3}{5} N \epsilon_F.$$

(b) Derive that the relation connecting the pressure and volume of an electron gas at 0 K is $p = (2/3)U_0/V$.

(c) Show that the bulk modulus $B = -V(\partial p / \partial V)$ of an electron gas at 0 K is $B = 5p/3 = 10U_0/9V$.

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Problema 4   *Thermal expansion influence on the free-electron gas*

Consider a sample of volume V containing N free electrons, where V experiences a thermal expansion given by $V = V_0(1 + \alpha T)$, with α as the volumetric thermal expansion coefficient. Considering such expansion on the volume, obtain the following quantities:

(a) The chemical potential $\mu(T)$,

$$\mu(T) = \epsilon_F (1 + \alpha T)^{-2/3} \left[1 - \frac{\pi^2}{12} \frac{(k_B T)^2}{\epsilon_F^2} \right].$$

with ϵ_F the Fermi energy.

(b) The kinetic energy $U(T)$,

$$U(T) = \frac{3}{5} N \epsilon_F (1 + \alpha T)^{-2/3} \left[1 + \frac{5\pi^2}{12} \frac{(k_B T)^2}{\epsilon_F^2} \right].$$

(c) The specific heat $c = C/N$, considering that $\alpha T \ll 1$,

$$c(T) = -\frac{2}{5} \alpha k_B T_F + \frac{2}{3} \alpha^2 k_B T_F T + \frac{\pi^2}{2} \frac{k_B T}{T_F}$$

where $T_F = \epsilon_F / k_B$ is the Fermi temperature.

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