Infinite matter

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Studies of infinite matter

- For historical and pedagogical reasons we start with the electron gas in two and three dimensions
- Thereafter we discuss infinite nuclear matter

Electron gas and HF solution

The electron gas is perhaps the only realistic model of a system of many interacting particles that allows for a solution of the Hartree-Fock equations on a closed form. Furthermore, to first order in the interaction, one can also compute on a closed form the total energy and several other properties of a many-particle systems. The model gives a very good approximation to the properties of valence electrons in metals. The assumptions are

- System of electrons that is not influenced by external forces except by an attraction provided by a uniform background of ions. These ions give rise to a uniform background charge. The ions are stationary.
- The system as a whole is neutral.
- We assume we have N_e electrons in a cubic box of length L and volume $\Omega = L^3$. This volume contains also a

uniform distribution of positive charge with density $N_e e/\Omega$.
This is a homogeneous system and the one-particle wave functions

Electron gas and HF solution

In exercise 5 we show that the Hartree-Fock energy can be written as

$$\varepsilon_k^{HF} = \frac{\hbar^2 k^2}{2m_e} - \frac{e^2}{\Omega^2} \sum_{k' \le k_F} \int d\mathbf{r} e^{i(\mathbf{k}'-\mathbf{k})\mathbf{r}} \int d\mathbf{r}' \frac{e^{i(\mathbf{k}-\mathbf{k}')\mathbf{r}'}}{|\mathbf{r}-\mathbf{r}'|}$$

resulting in

$$\varepsilon_k^{HF} = \frac{\hbar^2 k^2}{2m_e} - \frac{e^2 k_F}{2\pi} \left[2 + \frac{k_F^2 - k^2}{k k_F} ln \left| \frac{k + k_F}{k - k_F} \right| \right]$$

The results can be rewritten in terms of the density

$$n = \frac{k_F^3}{3\pi^2} = \frac{3}{4\pi r_s^3},$$

where $n = N_e/\Omega$, N_e being the number of electrons, and r_s is the radius of a sphere which represents the volum per conducting electron. It can be convenient to use the Bohr radius $a_0 = \hbar^2/e^2 m_e$. For most metals we have a relation $r_s/a_0 \sim 2-6$.

Exercises: Derivation of Hartree-Fock equations

Exercise 1

Consider a Slater determinant built up of single-particle orbitals ψ_λ, with $\lambda = 1, 2, \ldots, N$.
The unitary transformation

$$\psi_a = \sum_\lambda C_{a\lambda}\phi_\lambda,$$

brings us into the new basis. The new basis has quantum numbers $a = 1, 2, \ldots, N$. Show that the new basis is orthonormal. Show that the new Slater determinant constructed from the new single-particle wave functions can be written as the determinant based on the previous basis and the determinant of the matrix C. Show that the old and the new Slater determinants are equal up to a complex constant with absolute value unity. (Hint, C is a unitary matrix).

Exercises: Derivation of Hartree-Fock equations

Exercise 2

Consider the Slater determinant

$$\Phi_0 = \frac{1}{\sqrt{n!}} \sum_p (-)^p P \prod_{i=1}^{n} \psi_{\alpha_i}(x_i).$$

A small variation in this function is given by

$$\delta\Phi_0 = \frac{1}{\sqrt{n!}} \sum_p (-)^p P \psi_{\alpha_1}(x_1)\psi_{\alpha_2}(x_2)\dots\psi_{\alpha_{i-1}}(x_{i-1})(\delta\psi_{\alpha_i}(x_i))\psi_{\alpha_{i+1}}(x_{i+1}$$

Show that

$$\langle\delta\Phi_0|\sum_{i=1}^{n}\{t(x_i)+u(x_i)\}+\frac{1}{2}\sum_{i\neq j=1}^{n} v(x_i,x_j)|\Phi_0\rangle = \sum_{i=1}^{n}\langle\delta\psi_{\alpha_i}|\hat{t}+\hat{u}|\phi_{\alpha_i}\rangle + \sum_{i\neq j}^{n}$$

Exercises: Derivation of Hartree-Fock equations

Exercise 3

What is the diagrammatic representation of the HF equation?

$$-\langle \alpha_k | u^{HF} | \alpha_i \rangle + \sum_{j=1}^{n} [\langle \alpha_k \alpha_j | \hat{v} | \alpha_i \alpha_j \rangle - \langle \alpha_k \alpha_j | v | \alpha_j \alpha_i \rangle] = 0$$

(Represent $(-u^{HF})$ by the symbol $- - -$X .)

Exercises: Derivation of Hartree-Fock equations

Exercise 4

Consider the ground state $|\Phi\rangle$ of a bound many-particle system of fermions. Assume that we remove one particle from the single-particle state λ and that our system ends in a new state $|\Phi_n\rangle$. Define the energy needed to remove this particle as

$$E_\lambda = \sum_n |\langle \Phi_n | a_\lambda | \Phi \rangle|^2 (E_0 - E_n),$$

where E_0 and E_n are the ground state energies of the states $|\Phi\rangle$ and $|\Phi_n\rangle$, respectively.

- Show that

$$E_\lambda = \langle \Phi | a_\lambda^\dagger \left[a_\lambda, H \right] | \Phi \rangle,$$

where H is the Hamiltonian of this system.

- If we assume that Φ is the Hartree-Fock result, find the

relation between E_λ and the single-particle energy ε_λ for states $\lambda \leq F$ and $\lambda > F$, with

Exercises: Electron gas

Exercise 5

The electron gas model allows closed form solutions for quantities like the single-particle Hartree-Fock energy. The latter quantity is given by the following expression

$$\varepsilon_k^{HF} = \frac{\hbar^2 k^2}{2m} - \frac{e^2}{V^2} \sum_{k' \leq k_F} \int d\mathbf{r} e^{i(\mathbf{k}' - \mathbf{k})\mathbf{r}} \int d\mathbf{r}' \frac{e^{i(\mathbf{k} - \mathbf{k}')\mathbf{r}'}}{|\mathbf{r} - \mathbf{r}'|}$$

- Show that

$$\varepsilon_k^{HF} = \frac{\hbar^2 k^2}{2m} - \frac{e^2 k_F}{2\pi} \left[2 + \frac{k_F^2 - k^2}{k k_F} ln \left| \frac{k + k_F}{k - k_F} \right| \right]$$

(Hint: Introduce the convergence factor $e^{-\mu|\mathbf{r}-\mathbf{r}'|}$ in the potential and use $\sum_{\mathbf{k}} \rightarrow \frac{V}{(2\pi)^3} \int d\mathbf{k}$)

- Rewrite the above result as a function of the density

$$n = \frac{k_F^3}{3\pi^2} = \frac{3}{4\pi r_s^3},$$

Exercises: Electron gas

Solution to exercise 5

We want to show that, given the Hartree-Fock equation for the electron gas

$$\varepsilon_k^{HF} = \frac{\hbar^2 k^2}{2m} - \frac{e^2}{V^2} \sum_{p \leq k_F} \int d\mathbf{r} \exp\left(i(\mathbf{p}-\mathbf{k})\mathbf{r}\right) \int d\mathbf{r}' \frac{\exp\left(i(\mathbf{k}-\mathbf{p})\mathbf{r}'\right)}{|\mathbf{r}-\mathbf{r}'|}$$

the single-particle energy can be written as

$$\varepsilon_k^{HF} = \frac{\hbar^2 k^2}{2m} - \frac{e^2 k_F}{2\pi} \left[2 + \frac{k_F^2 - k^2}{k k_F} ln \left| \frac{k + k_F}{k - k_F} \right| \right].$$

We introduce the convergence factor $e^{-\mu|\mathbf{r}-\mathbf{r}'|}$ in the potential and use $\sum_{\mathbf{k}} \rightarrow \frac{V}{(2\pi)^3} \int d\mathbf{k}$. We can then rewrite the integral as

$$\frac{e^2}{V^2} \sum_{k' \leq k_F} \int d\mathbf{r} \exp\left(i(\mathbf{k}'-\mathbf{k})\mathbf{r}\right) \int d\mathbf{r}' \frac{\exp\left(i(\mathbf{k}-\mathbf{p})\mathbf{r}'\right)}{|\mathbf{r}-\mathbf{r}'|} = \frac{e^2}{V(2\pi)^3} \int d\mathbf{r} \int$$

and introducing the abovementioned convergence factor we have

Exercises: Electron gas

Exercise 6

We consider a system of electrons in infinite matter, the so-called electron gas. This is a homogeneous system and the one-particle states are given by plane wave function normalized to a volume Ω for a box with length L (the limit $L \to \infty$ is to be taken after we have computed various expectation values)

$$\psi_{\mathbf{k}\sigma}(\mathbf{r}) = \frac{1}{\sqrt{\Omega}} \exp{(i\mathbf{kr})}\xi_{\sigma}$$

where $\mathbf{k}$ is the wave number and ξ_{σ} is a spin function for either spin up or down

$$\xi_{\sigma=+1/2} = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \quad \xi_{\sigma=-1/2} = \begin{pmatrix} 0 \\ 1 \end{pmatrix}.$$

We assume that we have periodic boundary conditions which limit the allowed wave numbers to

$$k_i = \frac{2\pi n_i}{L} \quad i = x, y, z \quad n_i = 0, \pm 1, \pm 2$$

Exercises: Electron gas

Solution to exercise 6

We have to show first that

$$\hat{H}_b = \frac{e^2}{2}\frac{N_e^2}{\Omega}\frac{4\pi}{\mu^2},$$

and

$$\hat{H}_{el-b} = -e^2\frac{N_e^2}{\Omega}\frac{4\pi}{\mu^2}.$$

And then that the final Hamiltonian can be written as

$$H = H_0 + H_I,$$

with

$$H_0 = \sum_{\mathbf{k}\sigma}\frac{\hbar^2 k^2}{2m_e}a^\dagger_{\mathbf{k}\sigma}a_{\mathbf{k}\sigma},$$

and

$$H_I = \frac{e^2}{2\Omega}\sum\sum\frac{4\pi}{q^2}a^\dagger_{\mathbf{k}+\mathbf{q},\sigma_1}a^\dagger_{\mathbf{p}-\mathbf{q},\sigma_2}a_{\mathbf{p}\sigma_2}a_{\mathbf{k}\sigma_1}.$$

Electron gas and HF solution

Let us now calculate the following part of the Hamiltonian

$$\hat{H}_b = \frac{e^2}{2} \iint \frac{n(\mathbf{r})n(\mathbf{r}')e^{-\mu|\mathbf{r}-\mathbf{r}'|}}{|\mathbf{r}-\mathbf{r}'|} d\mathbf{r}d\mathbf{r}',$$

where $n(\mathbf{r}) = N_e/\Omega$, the density of the positive background charge. We define $\mathbf{r}_{12} = \mathbf{r} - \mathbf{r}'$, resulting in $d\mathbf{r}_{12} = d\mathbf{r}$, and allowing us to rewrite the integral as

$$\hat{H}_b = \frac{e^2 N_e^2}{2\Omega^2} \iint \frac{e^{-\mu|\mathbf{r}_{12}|}}{|\mathbf{r}_{12}|} d\mathbf{r}_{12} d\mathbf{r}' = \frac{e^2 N_e^2}{2\Omega} \int \frac{e^{-\mu|\mathbf{r}_{12}|}}{|\mathbf{r}_{12}|} d\mathbf{r}_{12}.$$

Here we have used that $\int \mathbf{r} = \Omega$. We change to spherical coordinates and the lack of angle dependencies yields a factor 4π, resulting in

$$\hat{H}_b = \frac{4\pi e^2 N_e^2}{2\Omega} \int_0^\infty r e^{-\mu r} \, \mathrm{d}r.$$

Solving by partial integration