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EXACT HARTREE-FOCK THEORY FOR A FERMION GAS IN THE JELLIUM MODEL

A, Cabrera, M.A. Ortíz, A. Calles and R.M. Méndez-Moreno

Departamento de Física, Facultad de Ciencias, UNAM
Apartado Postal 70-646, 04510 México, D.F.

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ABSTRACT

We propose a method for obtaining a formal analytical exact Hartree-Fock solution for a system of interacting fermions in the jellium model. The Hartree-Fock orbitals are expanded in terms of a basis of functions which have a continuous index. Then we obtain the algebraic Hartree-Fock equations for the coefficients in this expansion and it is shown that they satisfy a non linear, Fredholm, homogeneous integral equation of the second kind. Equations of this type are well known and there are several methods to solve them. Thus we claim that our problem can, in principle, be solved. A brief discussion of some methods for solving these equations is also presented.

RESUMEN

Se propone un método para obtener analíticamente una solución Hartree-Fock formal exacta, para un sistema de fermiones que interaccionan, en el modelo de jalea. Los orbitales Hartree-Fock se desarrollan en términos de una base de funciones que tienen un índice continuo. Se obtienen las ecuaciones algebraicas de Hartree-Fock para los coeficientes de este desarrollo y se demuestra que satisfacen una ecuación integral, no lineal, homogénea, de Fredholm de segunda clase.

Estas ecuaciones son bien conocidas y existen varios métodos para resolverlas. Por lo tanto afirmamos que, en principio, el problema está resuelto. Se presenta también una breve discusión de algunos métodos para resolver estas ecuaciones.

1. INTRODUCTION

The interacting fermion gas in the jellium model is a simple and successful model which finds applications in many branches of physics. For example it has been extensively used in Nuclear Physics[1] and in Solid State Physics.[2] This model lets us evaluate properties of many body systems (in the case of zero temperature as well as in the finite temperature regime); for example ground state energies, specific heats, bulk modulus and so on. In order to explicitely calculate some of these properties it is usual to begin with first order perturbation theory or whith the Hartree-Fock (HF) approximation. In the latter case there are many solutions to the HF equation in the zero temperature limit; for example the trivial solution plane waves[3] and the periodic waves of the type introduced by Overhauser[4] for the electron gas. These periodic solutions, called charge density waves, are found to be better than those of plane waves in the low density region[5]. This result is related with the Wigner's prediction about the electron gas cristalization[6]. The charge density waves are useful to evaluate physical properties of the many body systems, but an anlytical exact HF solution for these systems is still lacking.

In this work we propose a method for obtaining, in a systematic way, an analytic self-consistent HF solution for the ground state of the interacting fermion gas in the deformable jellium model. First of all, we expand the HF orbitals in terms of a basis with a continuos index.

We select this basis in such a way that we can easily reproduce some properties of the many fermion system; for example the energy at the low density regime. The proposition of expandind the HF orbitals in terms of a continuous basis has already been done for a system of fermions in the jellium model, interacting via interactions[7,8] (in the general three-dimensional case). We use the variational principle and find that the algebraic equations which determine the coefficients in the expansion lead to integral equations. This equations have been widely studied and there are methods to solve them. We discuss the difficulties which we found in the process of getting a solution in terms of a continuous basis and finally we comment about some of the methods which we chose to solve the integral equations.

2. ALGEBRAIC HF EQUATIONS FOR CONTINUOS STATES

The Hamiltonian for the fermion gas in the jellium model is

$$\hat{H} = \hat{H}_p + \hat{H}_b + \hat{V}_{bp} \quad , \tag{1}$$

where, as usual

$$\hat{H}_p = \sum_{i=1}^{N} \frac{p_i^2}{2m} + \frac{1}{2} \sum_{i \neq j}^{N} V(\underline{r}_i - \underline{r}_j) = \hat{T} + \hat{V} \quad ,$$

$$\hat{H}_b = \hat{V}_{bb} = \frac{1}{2} \iint N(\underline{R})\, N(\underline{R}')\, V(\underline{R} - \underline{R}')\, d^3R\, d^3R' \quad ,$$

$$\hat{V}_{bp} = - \sum_{i=1}^{N} \int N(\underline{R})\, V(\underline{r}_i - \underline{R})\, d^3R \quad ,$$

and $N(\underline{R})$ is the background density.

As it is known, it has been proved that in the independent particle model an in the deformable jellium model (where the background deforms in order to obtain the minimum energy) the expresion for the ground state energy reduces to[9]

$$E = \sum_{\underline{k}_1}^{\underline{k}_f} \sum_{\lambda_1 \lambda_2} \delta_{\lambda_1 \lambda_2} \langle \underline{k}_1 \lambda_1 | \hat{T} | \underline{k}_1 \lambda_2 \rangle - \frac{1}{2} \sum_{\underline{k}_1 \neq \underline{k}_2}^{\underline{k}_f} \sum_{\lambda_1 \lambda_2} \langle \underline{k}_1 \lambda_1, \underline{k}_2 \lambda_2 | \hat{V} | \underline{k}_2 \lambda_2, \underline{k}_1 \lambda_1 \rangle \tag{2}$$

this is because the energy of the two background terms cancels out identically with the direct part of the particle-particle interaction.

We propose to expand the orbitals in terms of a basis with a continuous index, so the spin orbitals are

$$\psi_{\underline{k}\lambda}(\underline{r}) = \eta_\lambda \, \phi_{\underline{k}}(\underline{r}) = \eta_\lambda \int C_{\underline{k}}(\underline{q}) \, |\underline{q}, \underline{r}> d^3q \quad , \tag{3}$$

where η_λ are the spin functions.

Then from Eqs. (2) and the proposition given by Eqs. (3), the energy can be written as

$$E = \sum_{\underline{k}_1}^{\underline{k}_f} \sum_{\lambda_1} \iint C^*_{\underline{k}_1}(\underline{q}_1) <q_1|\hat{T}|q_3> C_{\underline{k}_1}(\underline{q}_3) \, \eta^+_{\lambda_1}\eta_{\lambda_1} d^3q_1 d^3q_3$$

$$- \frac{1}{2} \sum_{\underline{k}_1 \neq \underline{k}_2}^{\underline{k}_f} \sum_{\lambda_1,\lambda_2} \iiiint C^*_{\underline{k}_1}(\underline{q}_1) C^*_{\underline{k}_2}(\underline{q}_2) <\underline{q}_1\underline{q}_2|\hat{V}|\underline{q}_4\underline{q}_3> C_{\underline{k}_2}(\underline{q}_4) C_{\underline{k}_1}(\underline{q}_3) \delta_{\lambda_1\lambda_2} \, \eta^+_{\lambda_1}\eta_{\lambda_2} \cdot$$

$$\cdot \, d^3q_1 d^3q_2 d^3q_3 d^3q_4 \, , \tag{4}$$

where the brackets $<\underline{q}_i|\hat{F}|\underline{q}_j> = \int \phi^*_{\underline{q}_i}(\underline{r}) \, \hat{F}\phi_{\underline{q}_j}(\underline{r}) \, d^3r$.

Making the variation to first order in the coefficients of the expansion, with the normalization condition

$$<\underline{k}_1|\underline{k}_1> = \sum_{\lambda_1} \int C^*_{\underline{k}_1}(\underline{q}_1) <q_1|\underline{q}_3> C_{\underline{k}_1}(\underline{q}_3) \, d^3q_1 d^3q_3 \eta^+_{\lambda_1}\eta_{\lambda_1}$$

$$= \sum_{\lambda_1} \eta^+_{\lambda_1}\eta_{\lambda_1} \int C^*_{\underline{k}_1}(\underline{q}_1) C_{\underline{k}_1}(\underline{q}_1) \, d^3q_1 = 1 \quad ,$$

we obtain

$$\sum_{\underline{k}_1}^{\underline{k}_f} \sum_{\lambda_1} \iint \delta_{\underline{k}_1\underline{k}} \delta_{\underline{q}_1\underline{q}} <q_1|\hat{T}|q_3> C_{\underline{k}_1}(q_3) d^3\underline{q}_1 d^3\underline{q}_3 \, \eta^+_{\lambda_1}\eta_{\lambda_1}$$

$$- \sum_{\underline{k}_1 \neq \underline{k}_2}^{\underline{k}_f} \sum_{\lambda_1,\lambda_2} \iiiint \delta_{\underline{k}_1\underline{k}} \delta_{q_1 q} C^*_{\underline{k}_2}(\underline{q}_2) <\underline{q}_1\underline{q}_2|\hat{V}|\underline{q}_4\underline{q}_3> C_{\underline{k}_2}(\underline{q}_4) C_{\underline{k}_1}(\underline{q}_3) \cdot$$

$$\cdot \, \delta_{\lambda_1\lambda_2} \, \eta^+_{\lambda_1}\eta_{\lambda_2} d^3q_1 d^3q_2 d^3q_3 d^3q_4 = \sum_{\underline{k}_1}^{\underline{k}_f} \sum_{\lambda_1} \int \delta_{\underline{k}_1\underline{k}} \delta_{\underline{q}_1\underline{q}} C_{\underline{k}_1}(\underline{q}_1) d^3q_1 \, \eta^+_{\lambda_1}\eta_{\lambda_1} \cdot$$

This equation gives us the next condition:

$$\int \left\{ \langle \underline{q}_1 | \hat{T} | \underline{q}_3 \rangle - \int \sum_{\underline{k}_2}^{\underline{k}_f} C^*_{\underline{k}_2}(\underline{q}_2) \langle \underline{q}_1 \underline{q}_2 | \hat{V} | \underline{q}_4 \underline{q}_3 \rangle C_{\underline{k}_2}(\underline{q}_4) d^3q_2 d^3q_4 \right\} C_{\underline{k}}(\underline{q}_3)\, d^3q_3 \tag{6}$$

$$= \varepsilon_{\underline{k}}\, C_{\underline{k}}(\underline{q}_1)$$

We have a non linear, homogeneous, integral equation of third order in the coefficients $C_{\underline{k}}$. We propose to identify the Kernel of this equation as a function of some of the coefficients $C_{\underline{k}}$, then

$$k(\underline{q}_1, \underline{q}_3, c) = \langle \underline{q}_1 | \hat{T} | \underline{q}_3 \rangle - \int \sum_{\underline{k}_2}^{\underline{k}_f} C^*_{\underline{k}_2}(\underline{q}_2) \langle \underline{q}_1 \underline{q}_2 | \hat{V} | \underline{q}_4 \underline{q}_3 \rangle C_{\underline{k}_2}(\underline{q}_4) d^3q_2 d^3q_4 , \tag{7}$$

and with this proposition we can write Eq. (6) as

$$\int K(\underline{q}_1, \underline{q}_3, c)\, C_{\underline{k}}(\underline{q}_3)\, d^3q_3 = \varepsilon_{\underline{k}} C_{\underline{k}}(\underline{q}_1) \ . \tag{8}$$

This equation is well known. It is a homogeneous, non-linear, Fredholm integral equation of second kind. There are many methods for obtaining approximated solutions to this type of equations; for example Ritz's method, the Trace's method and Kellog's method[10,11].

With this identification of our equation we have reduce the problem to a known one. Fortunatelly there are theorems concerning the convergence of this type of equations, however as these are not linear equations we have not theorems about unicity of the solutions.

We remark that handling this equation in an appropiate way is very cumbersome because the index $\underline{k}$ is a continuous one. Next we discuss the difficulties which appear and the methods that we propose to obtain a solution for the HF equations.

DISCUSSION

Among the methods found in the literature to solve Eq. (8) we selected Ritz's method because it was the way followed by C.C. J. Roothaan to get solutions for the HF albegraic equations for finite systems.[12] The Ritz method gives us the coefficients $C_{\underline{k}}(\underline{q})$ in the

in the approximation we require and the efficiency of this has been widely shown.

The function $C_{\underline{k}}(\underline{q})$ is expanded in terms of a basis with a discret index

$$C_{\underline{k}}(\underline{q}) = \sum_n a_n^{\underline{k}} f_n(\underline{q}) \quad . \tag{9}$$

This expansion is introduced in the equation which defines the function $K(\underline{q}_1, \underline{q}_3\ C)$, and this function is substitued in Eq. (8). Multiplying Eq. (8) by $f^*_m(\underline{q})$ and integrating with respect to $\underline{q}$ we obtain the self-consistent, matricial equation of eigenvalues

$$\sum_n \langle \psi_m(\underline{q}_1) | K(\underline{q}_1, \underline{q}_3, a) | \psi_n(\underline{q}_1) \rangle a_n^{\underline{k}} = \varepsilon_{\underline{k}}\, a_m^{\underline{k}} \quad . \tag{10}$$

To solve this equation we give initial values for the coefficients $a_n^{\underline{k}}$ in the function $K[\underline{q}_1, \underline{q}_3, C(a,\underline{q})]$ and with the usual techniques we get a solution to the resulting eigenvalues equation. The eigenvector obtained is substituted in the Kernel of Eq. (10). This equation is solved again yielding a new eigenvector. We repeat this procedure iteratively until self-consistency is achieved up to a given accuracy.

The coefficients $a_n^{\underline{k}}$ are functions of the discrete index n, and the continuous index $\underline{k}$. The dependence on the continuous index $\underline{k}$ obviously introduces serious difficulties, because the infinite number of equations involved. In order to solve these difficulties we propose two methods: in the first one we separate the dependence of the coefficients on the index $\underline{k}$ from the dependence on the discrete index n, *i.e.*, $a_n^{\underline{k}} = b^{\underline{k}} b_n$, this kinds of separation allows us to handle the equations, numerically, for the coefficients $a_n^{\underline{k}}$ along with the corresponding diagonalization and self-consistency.

In the second method we consider the index $\underline{k}$ as a continuous variable all the time and we propose an expansion in a six dimensional basis, three dimensions for the coordinates $\underline{r}$ and the other three for the components of the vector $\underline{k}$. This is done instead of the usual expansion in a three dimensional basis. There are references about the utilization

of basis with more than three dimensions.[13] Following this procedure we can get a solution to our equations.

In this way we have shown how one can get solutions to the HF equations for a three dimensional gas of interacting fermions in the deformable jellium model. The type of basis we choose in our expansions will depend on the kind of interactions between the particles and on the properties of the system which we are interested in reproducing.

This method provides a systematic way for obtaining algebraic self-consistent H.F. solutions for the systems here considered and we hope that this will encourage further research on systems of many fermions, using solutions of the type considered in this work.

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