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A THEOREM ON THE JELLIUM MODEL

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ABSTRACT

Starting with the jellium model we apply a variational principle varying the background density. As a result we get general conditions on the background density allowing new physical meaning to the jellium model. As a particular case, when we use an independent particle state function, we obtain the usual assumptions used to define the "deformable jellium model".

RESUMEN

A partir del modelo de jalea aplicamos un principio variacional cambiando la densidad de fondo. Como resultado obtenemos condiciones generales sobre dicha densidad, lo cual le da un nuevo significado físico al modelo de jalea. Como un caso particular, cuando usamos una función de estado de partícula independiente, obtenemos las hipótesis usuales que se utilizan para definir el "modelo de jalea deformable".

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INTRODUCTION

The models of particle gases have been very useful in describing approximately several physical phenomena such as: conduction in metals, properties of plasma and nuclear matter, Wigner cristalization in electron gases, etc.[1,2]. In the description of charged particle gases, a charged background is frequently introduced to assure the neutrality of the total system, the background is inert and the energy of the system is finite. The model is called "jellium model"[2]. In case the background deforms in order to produce local neutrality, the model is called "deformable jellium model"[3,4]. The usual description of this last model is worked out in the Hartree-Fock approximation. Here the background has not kinetic energy and it is constructed in such a way that the background-background energy, the particle-background energy and the direct term cancel each other exactly. In this work we show among other things that the last assumption is obtained from a variational principle when it is applied to an independent particle state function.

THE THEOREM

Let us consider the system of N particles whose Hamiltonian is written as

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

where

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

$$\hat{H}_b = \hat{V}_{bb} = \frac{1}{2} \int n(\underline{R}) n(\underline{R}') V(\underline{R}, \underline{R}') d\underline{R}\, d\underline{R}' \tag{1b}$$

and

$$\hat{V}_{pb} = - \sum_{i=1}^{N} \int n(\underline{R}) V(\underline{r}_i, \underline{R}) d\underline{R} \quad . \tag{1c}$$

Here $n(R)$ is the background density, $\hat{H}_p$ is the particle Hamiltonian, $\hat{H}_b$ is the background Hamiltonian, $\hat{V}_{bp}$ is the particle-background interaction, and the interaction V in (1a), (1b) and (1c) is supposed to be the same. We are interested in the value of the ground state energy with the state function ψ.

The optimum energy, at first order variation in $n(R)$, is obtained when it satisfies

$$\int n(\underline{R})V(\underline{R},X)d\underline{R} = \sum_{i=1}^{N} \langle \psi | V(\underline{r}_i,\underline{X}) | \psi \rangle \quad .$$

Proof:

The energy of the system is

$$E = \langle \psi | H | \psi \rangle = \langle \psi | H_p | \psi \rangle + \langle \psi | V_{bp} | \psi \rangle + V_{bb} = \sum_{i=1}^{N} \langle \psi | T(\underline{r}_i) | \psi \rangle +$$

$$+ \frac{1}{2} \sum_{i \neq j}^{N} \langle \psi | V(\underline{r}_i,\underline{r}_j) | \psi \rangle - \sum_{i=1}^{N} \int \langle \psi | n(\underline{R}) V(\underline{r}_i,\underline{R}) | \psi \rangle d\underline{R} +$$

$$+ \frac{1}{2} \iint n(\underline{R}) n(\underline{R}') V(\underline{R},\underline{R}') d\underline{R}\, d\underline{R}' \quad . \qquad (2)$$

This energy depends on the background distribution. In order to obtain the optimum energy we perform the first order variation.

The application of the Hellman-Feynman[5] theorem to Eq. (2) gives us

$$\frac{\partial E}{\partial n(\underline{X})} = -\sum_{i=1}^{N} \langle \psi | \int \frac{\partial n(\underline{R})}{\partial n(\underline{X})} V(\underline{r}_i,\underline{R}) d\underline{R} | \psi \rangle + \iint \frac{\partial n(\underline{R})}{\partial n(\underline{X})} n(\underline{R}') V(\underline{R},\underline{R}') d\underline{R}\, d\underline{R}' \quad , \qquad (3)$$

which reduces to

$$\int n(\underline{R}')V(\underline{X},\underline{R}')d\underline{R}' = \sum_{i=1}^{N} \langle \psi | V(\underline{r}_i,\underline{X}) | \psi \rangle \quad . \qquad (4)$$

This equation is the condition we were looking for in order to prove the theorem.

Let us analyze some implications of the theorem. Using Eq. (4) the energy becomes

$$E = \sum_{i=1}^{N} \langle\psi|T(\underline{r}_i)|\psi\rangle + \frac{1}{2}\sum_{i\neq j}^{N} \langle\psi|V(\underline{r}_i,\underline{r}_j)|\psi\rangle -$$

$$- \sum \langle\psi| \left\{ \sum \langle\psi'|V(\underline{r}'_j,\underline{r}_i)|\psi'\rangle \right\} |\psi\rangle +$$

$$+ \frac{1}{2}\sum_{i\neq j}^{N} \langle\psi| \left\{ \langle\psi'|V(\underline{r}_i,\underline{r}'_j)|\psi'\rangle \right\} |\psi\rangle \quad ,$$

which reduces to

$$E = \sum_{i=1}^{N} \langle\psi|T(\underline{r}_i)|\psi\rangle + \frac{1}{2}\sum_{i\neq j}^{N} \langle\psi|V(\underline{r}_i,\underline{r}_j)|\psi\rangle -$$

$$- \frac{1}{2}\sum_{i\neq j}^{N} \langle\psi\psi'|V(\underline{r}_i,\underline{r}'_j)|\psi\psi'\rangle \quad . \tag{5}$$

Now let us assume the particles are fermions and the solution is written in the independent particle approximation, then

$$\psi = \frac{1}{\sqrt{N!}} \det \left[\varphi_{\underline{n}_i}(\underline{r}_i) \right] \quad , \tag{6}$$

with the orthonormalized spin-orbitals

$$\varphi_{\underline{n}_i}(\underline{r}_i) = \varphi_{n_i l_i m_i}(\underline{r}_i)\chi_{\sigma_i} = |\underline{n}_i\rangle \quad .$$

Using Eq. (6) the expression for the ground state energy (Eq. (5)) can be written as

$$E = \sum_{i=1}^{N} \langle\underline{n}_i|T(\underline{r})|\underline{n}_i\rangle + \frac{1}{2}\sum_{i\neq j}^{N} \langle\underline{n}_i\,\underline{n}_j|V(\underline{r},\underline{r}')|\underline{n}_i\,\underline{n}_j\rangle -$$

$$- \frac{1}{2}\sum_{i\neq j}^{N} \langle n_i\, n_j|V(\underline{r},\underline{r}')|n_j\, n_i\rangle - \frac{1}{2}\sum_{i\neq j}^{N} \langle\underline{n}_i\,\underline{n}_j|V(\underline{r},\underline{r}')|\underline{n}_i\,\underline{n}_j\rangle \quad , \tag{7}$$

where the last term is the negative of the direct term, and thus

$$E = \sum_{i=1}^{N} \langle \underline{n}_i | T(\underline{r}) | \underline{n}_i \rangle - \frac{1}{2} \sum_{i \neq j}^{N} \langle \underline{n}_i \underline{n}_j | V(\underline{r},\underline{r}') | \underline{n}_j \underline{n}_i \rangle \quad ; \qquad (8)$$

the energy of the system is the sum of the kinetic energy and the exchange term. Subsequently, the orbitals are optimized to obtain the best energy, resulting in the Hartree-Fock equations, but in this case reduced as in Eq. (8), where the direct, background-background and background-particle terms in Eq. (7) have been cancelated; that is

$$\langle \hat{V}_d \rangle + \langle \hat{V}_{bb} \rangle + \langle \hat{V}_{bp} \rangle = 0 \quad .$$

In the independent particle approximation the condition for the density $n(R)$ in Eq. (4) reduces to

$$\int n(\underline{R}') \, V(\underline{X},\underline{R}') \, \underline{d}R' = \sum_{i=1}^{N} \int \varphi_{\underline{n}_i}^{*}(\underline{r}) \, V(\underline{r},\underline{X}) \, \varphi_{\underline{n}_i}(\underline{r}) \, d\underline{R} \quad . \qquad (9)$$

A particular solution to this equation is

$$n(\underline{R}) = \sum_{i=1}^{N} \varphi_{\underline{n}_i}^{*}(\underline{R}) \, \varphi_{\underline{n}_i}(\underline{R}) \quad , \qquad (10)$$

which means that the "charged" background density deforms according to the particle density. This is the well known deformable jellium model[3].

It is worth while to note that the potential does not need to depend on the interparticle distances, neither on the form of the interaction, as it has been used in the literature.

CONCLUSIONS

Using the condition that the potentials in Eqs. (1a), (1b) and (1c) are all the same, we found Eq. (4) as the background "charge" distribution which gives the best energy for the system. This result does not depend on the potential neither on the state function, provided the Hellman-Feynman theorem could be applied. In this general case, Eq. (4) implies in the energy Eq. (5) that the background-background and particle-background terms add in a single term.

When ψ is an independent particle state function, the theorem

reproduces the usual deformable jellium model, so the use of HF approximation is not a necessary condition to work with the jellium model as it is well known.

The way we justified the deformable jellium model, in this paper, allows us to give further physical meaning to it. In this respect the physical arguments used by Overhauser[6] to support the model are well and formally established. What is new here is that we based on a variational principle the hypothesis or approximations claimed to define the model[7].

On the other hand, according with Eq. (5) when we are dealing with the exact solution, it is not clear at all how the cancellation of the energy terms occurs so the physical arguments that define the model are valid exactly only when independent particle state functions are used.

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