NOTE ON CORRELATION ENERGY OF THE ELECTRON GAS (*)

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ABSTRACT — An attempt has been made to describe the correlation structure of the electron gas in terms of the collective modes only. A very simple formalism is obtained which leads to very good agreement with the results of Nozières-Pines and Hubbard for low momentum transfer ($K/K_F < 1$), if one neglects the exchange terms.

The subject of this paper is a new interpretation of the electron gas correlation energy as the zero point energy of the collective degrees of freedom.

Our aproach is extremely simple and leads to close agreement with the well known results of NOZIÈRES & PINES (1) and of HUBBARD (2).

We must conclude that our assumptions are meaningful at least as far as long wavelength modes are concerned.

Let us consider the operators

$$A_k^+ = N_k \sum_q C_{q+k}^+ C_q \tag{1}$$

(suggested by Pines work) where q is such that $|q| < k_f$, $|q+k| > k_F$ and C^+, C are the fermion operators of the second quantization. C_{q+k}^+ is a creation operator which creates a particle of momentum $q+k$ and C_q is an annihilation operator that destroys a particle with momentum q.

The quantity N_k is determined by normalization. We obtain

$$N_k = \left[\frac{\Omega}{(2\pi)^2} k_F^3 \left(x - \frac{x^3}{12}\right)\right]^{-1/2} \tag{2}$$

where $x = k/k_F$ and k_F is the Fermi level momentum. Thus the operator A_k^+ when operating on the vacuum, $|>$, yields a state of momentum k denoted by $|k>$.

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The operators A_k^+, A_k satisfy the following commutation rules

$$\begin{aligned} [A_k, A_k^+] &= \delta_{kk'} \\ [A_k, A_{k'}] &= 0 \end{aligned} \tag{3}$$

We can justify these relations if we note, for instance, that

$$< | A_k^2 A_k^{+2} | > \simeq 2 \tag{4}$$

(the equality is obtained by adding to the r. h. s. a quantity that is inversely proportional to the number of particles), and if we compute $< | [A_k^2, A_k^{+2}] | >$ accepting (3) we obtain

$$< | A_k^2, A_k^{+2} | > = 2 \tag{5}$$

Thus A_k and A_k^+ must be understood as bosom operators. With the operators A_k and A_k^+ we can construct an hamiltonian which, up to terms quadratic in the boson operators, is equivalent to the exact hamiltonian

$$H = \sum_i \frac{p_i^2}{2m} + \sum_{i<j} v(r_{ij}) = T + V \tag{6}$$

The equivalent hamiltonian

$$H_{eq} = E_{HF} + \sum_k (e_k + g_k) A_k^+ A_k + \frac{1}{2} \sum_k g_k (A_k^+ A_{-k}^+ + A_{-k} A_k) \tag{7}$$

is constructed so that (6) and (7) have the same matrix elements, that is to say:

$$\begin{aligned} < | H_{eq} | > &= < | H | > = E_{HF} \\ < | A_k H_{eq} A_k^+ | > &= < | A_k H A_k^+ | > = E_{HF} + e_k + g_k \\ < | A_k A_{-k} H_{eq} | > &= < | A_k A_{-k} H | > = g_k \end{aligned} \tag{8}$$

E_{HF} is the Hartree Fock energy and

$$e_k = < | A_k T A_k^+ | > = \frac{\left(\frac{4}{3} \frac{k_F^2}{2m} x \right)}{\left(1 - \frac{x^2}{12} \right)} \tag{9}$$

The matrix element g_k has been computed neglecting the exange term and the Hartree Fock self consistent potencial and with $v(r_{ij}) = \frac{e^2}{r_{ij}}$

$$g_k = <| A_k \, V \, A_k^+ | > = \frac{\alpha \, r_s}{\pi \, m} \, k_F^2 \, \frac{1}{x} \left(1 - \frac{x^2}{12}\right) \tag{10}$$

where $me^2 / k_F = \alpha \, r_s$ and $\alpha = (4\pi/9)^{1/3}$.

The quantities (2) (9) and (10) are the results for $x < 2$. When $x > 2$ we obtain

$$N_k = \frac{2\,\Omega}{(2\pi)^3} \frac{4}{3} \pi \, k_F^3 \tag{11}$$

$$e_k = \frac{k_P^2}{2\,m} x^2 \tag{12}$$

$$g_k = \frac{4}{3} \frac{\alpha \, r_s}{\pi \, m} \, k_F^2 \, \frac{1}{x^2} \tag{13}$$

The hamiltonian H_{eq} can be diagonalized by the transformation

$$\begin{aligned} B_k^+ &= x_k \, A_k^+ - y_k \, A_{-k} \\ B_k &= x_k \, A_k - y_k \, A_{-k}^+ \end{aligned} \tag{14}$$

where x_k and y_k are real quantities, such that $x_k^2 - y_k^2 = 1$, which is the condition for the operators B_k, B_k^+ to obey boson comutations relations.

We denote the diagonalized hamiltonian by

$$H = E_{HF} + E_c + \sum_k w_k \, B_k^+ \, B_k \tag{15}$$

The equations of motion $[B_k^+, H] = w_k \, B_k^+$, $[B_k, H] = -w_k, B_k$ give

$$w_k = [e_k \, (e_k + 2\, g_k)]^{1/2} \tag{16}$$

$$E_c = \frac{1}{2} \sum_k (w_k - e_k - g_k) \tag{17}$$

We can convert the amount (17) to an integration over the interval $(0, \infty)$

$$E_c = \frac{1}{(\alpha \, r_s)^2} \, \frac{3}{4} \int_o^\infty x^2 \, (w_k(x) - e_k(x) - g_k(x)) \, dx \tag{18}$$

In fig. 1 we plot the integrand. We notice that our result are between Nozières-Pines and Hubbard results.

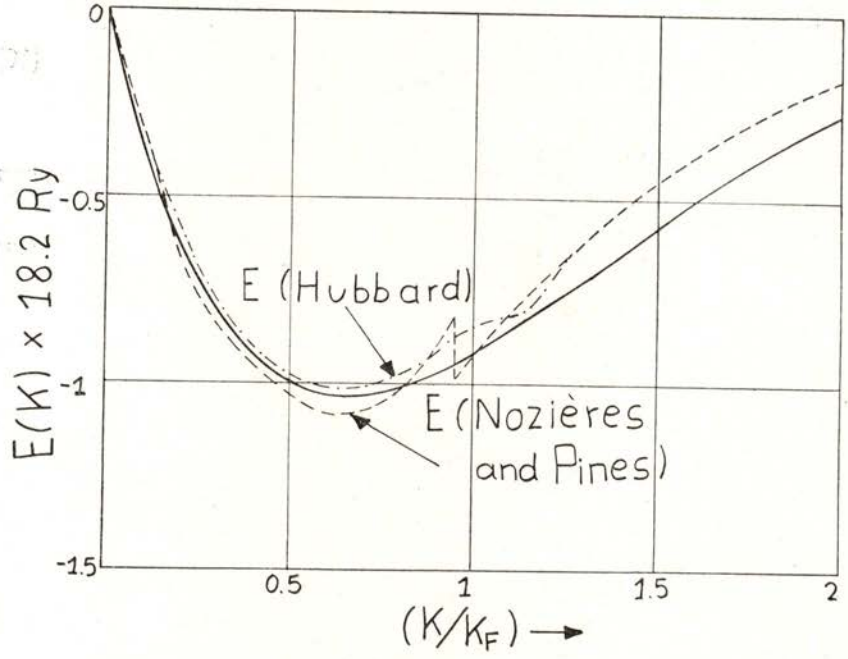

Fig. 1

The correlation energy may be considered as a sum of contributions from each value of k. For k such that $k/k_F < 1$ the collective modes described by the operators A_k, A_k^+ are responsable for nearly all the correlation energy.

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REFERENCES

(1) NOZIÈRES, P., & PINES, D. — *Phys. Rev.*, 111, 442, 1958.
(2) HUBBARD, J. — *Proc. Roy. Soc.* (London), A243.