A SIMPLIFIED VERSION OF THE RANDOM-PHASE APPROXIMATION AND THE PROBLEM OF THE CORRELATION ENERGY OF A MANY-FERMION SYSTEM (*)

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ABSTRACT — A discrepancy between the formula for the correlation energy of a many-fermion system derived by the conventional random phase approximation (RPA) method and the corresponding expression derived by summation of perturbation theory bubble diagrams is investigated.

It is shown that this discrepancy is absent from a simplified version of the RPA dealing only with collective excitations. As an example, the new version of the RPA is applied, with good results, to the electron gas.
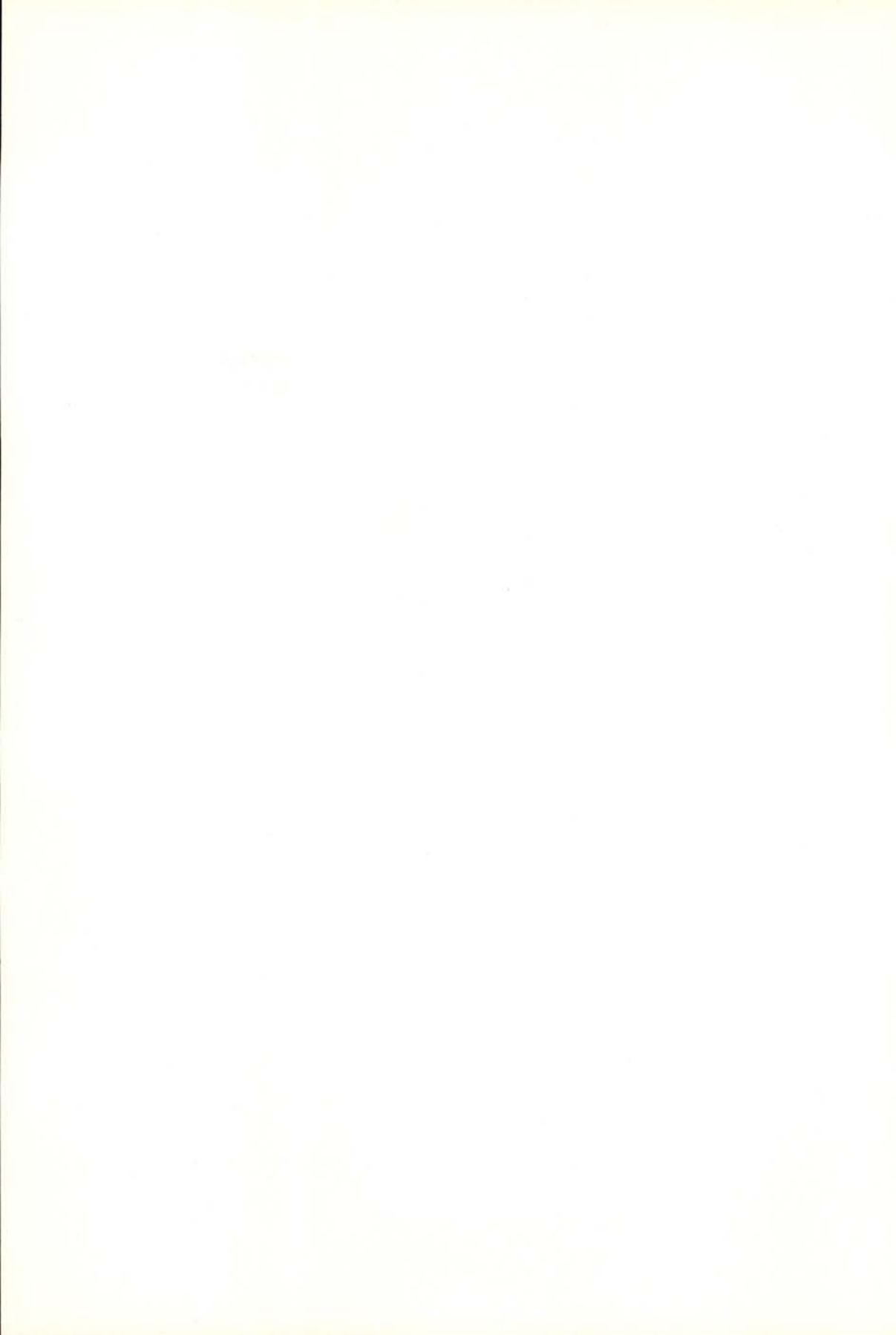
1 — INTRODUCTION

In this article we will develop some ideas which we have already presented, in a condensed form, in a previous publications (1). A more detailed account of the results of ref. 1 will also be given here. We discuss a type of discrepancy which may appear in calculations of correlation effects based on the random phase approximation (RPA). It is well known that an expression for the correlation energy of a many-fermion system arises naturally in the diagonalization of an effective boson hamiltonian obtained by the procedure which we now describe. Let

$$H = \sum_{ij} k_{i,j} \, c_i^+ \, c_j + \frac{1}{2} \sum_{ijkl} v_{ij,kl} \, c_i^+ \, c_j^+ \, c_l \, c_k \,, \qquad (1.1)$$

be the hamiltonian of some system. The c_i^+, c_j are fermion operators. We denote by the letters a, b, c, ... occupied single particle states in the Hartree-Fock ground state $|0>$ of our system and we denote by $m, n, p, ...$ non-occupied single particle states. A standard procedure (2) for arriving at the RPA is to replace pairs of fermion operators $c_a^+ \, c_m$ by true boson operators B_{ma},

$$c_a^+ \, c_m \rightarrow B_{ma} \,,$$
$$[B_{ma}, B_{nb}] = 0 \,, \quad [B_{ma}, B_{nb}^+] = \delta_{mn} \, \delta_{ab} \,. \qquad (1.2)$$

One then replaces the Hartree-Fock state $|0>$ by the boson vacuum $|0>$ and finally one replaces the hamiltonian H by a new hamiltonian H_B, quadratic in the boson operators, which one requires to be equivalent to H in the sense that

$$<0|H \, c_m^+ \, c_a|0> \, = \, <0|H_B \, B_{ma}^+|0> \,,$$
$$<0|c_b^+ \, c_n \, H \, c_m^+ \, c_a|0> \, = \, <0|B_{nb} \, H_B \, B_{ma}^+|0> \,,$$
$$<0|H \, c_n^+ \, c_b \, c_m^+ \, c_a|0> \, = \, <0|H_B \, B_{nb}^+ \, B_{ma}^+|0> \,. \qquad (1.3)$$

We then have (2)

$$H_B = E_{HF} + \sum (\varepsilon_m - \varepsilon_a) B_{ma}^+ B_{ma}$$
$$+ \sum (v_{an,mb} - v_{an,bm}) B_{nb}^+ B_{ma}$$
$$+ \frac{1}{2} \sum (v_{ab,mn} - v_{ab,nm}) B_{nb} B_{ma} \qquad (1.4)$$
$$+ \frac{1}{2} \sum (v_{mn,ab} - v_{mn,ba}) B_{nb}^+ B_{ma}^+$$

where the ε_i are Hartree-Fock single particle energies,

$$k_{i,j} + \sum_a (v_{ia,ja} - v_{ia,aj}) = \varepsilon_i \delta_{ij} , \qquad (1.5)$$

and E_{HF} is the Hartree-Fock ground state energy. The new hamiltonian can be diagonalized by a cannonical transformation

$$\theta_r^+ = \sum_{ma} (X_{ma}^{(r)} B_{ma}^+ + Y_{ma}^{(r)} B_{ma})$$
$$[\theta_r, \theta_s] = O, \quad [\theta_r, \theta_s^+] = \delta_{rs} . \qquad (1.6)$$

Indeed, H_B attains the form

$$H_B = E_{HF} + E_c + \sum_r \omega_r \theta_r^+ \theta_r , \qquad (1.7)$$

provided the amplitudes $X_{ma}^{(r)}$, $Y_{ma}^{(r)}$ satisfy the eigenvalue equations

$$(\varepsilon_m - \varepsilon_a) X_{ma}^{(r)} + \sum_{nb} [(v_{mb,an} - v_{mb,na}) X_{nb}^{(r)}$$
$$- (v_{mn,ab} - v_{mn,ba}) Y_{nb}^{(r)}] = \omega_r X_{ma}^{(r)}$$
$$(\varepsilon_m - \varepsilon_a) Y_{ma}^{(r)} + \sum_{nb} [(v_{an,mb} - v_{an,bm}) Y_{nb}^{(r)}$$
$$- (v_{ab,mn} - v_{ab,nm}) X_{nb}^{(r)}] = - \omega_r Y_{ma}^{(r)} . \qquad (1.8)$$

The quantities ω_r are excitation energies and E_c is the correlation energy. As a by product of the diagonalization of H_B one obtains the following expression for E_c

$$E_c = \frac{1}{2} \sum_r \omega_r - \frac{1}{2} \sum_{ma} (\varepsilon_m - \varepsilon_a + v_{am,ma} - v_{am,am}) . \qquad (1.9)$$

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Now this equation overestimates, by an ammount equal to the second order energy, the correlation energy obtained by summing the so called bubble diagrams. Indeed, the perturbation theory result is (3)

$$E_{c,\,PT} = \frac{1}{2} \sum_r \omega_r - \frac{1}{2} \sum_{ma} (\varepsilon_m - \varepsilon_a + v_{am,\,ma} - v_{am,\,am})$$
$$- \frac{1}{2} \sum_{abmn} \frac{v_{ab,\,mn} (v_{mn,\,ab} - v_{mn,\,ba})}{\varepsilon_a + \varepsilon_b - \varepsilon_m - \varepsilon_n} \quad . \tag{1.10}$$

We wish to investigate the discrepancy between eqs. (1.9) and (1.10). This discrepancy shows the RPA derivation of the correlation energy to be unsatisfactory. We must conclude therefore that some of the RPA assumptions are violated, i.e., some of the quantities

$$\sum_r (X_{ma}^{(r)^*} c_a^+ c_m + Y_{ma}^{(r)^*} c_m^+ c_a)$$

must fail to behave as boson operators. It has been conjectured that this discrepancy could be remedied by discarding the non-collective RPA modes (4) since one expects only the collective modes to behave as bosons. Then eq. (1.7) may be replaced by

$$H = H_{int} + \sum_r \omega_r \theta_r^+ \theta_r \tag{1.11}$$

where the summation extends only over collective modes and H_{int} *is* intrinsic in the sense that it commutes with collective operators θ_r. The expectation values of H_{int} already includes the contribution of the zero-point fluctuations of the collective modes to the correlation energy. One expects that correlation effects associated with the intrinsic degrees of freedom may be taken care of by low order perturbation theory, if necessary.

2. A VERSION OF THE RPA RESTRICTED TO COLLECTIVE EXCITATIONS

If we apply eq. (1.9) to the electron gas we obtain a divergent result. The divergency is removed by using eq. (1.10) instead of eq. (1.9). Since the discrepancy between the two equations is infinite for the electron gas, this system may be used as a convenient example to investigate the source of that discrepancy.

We develop now a version of the RPA dealing only with the collective degrees of freedom having mainly in mind the electron gas. The method may be easily extended to other systems and should be free of the inconsistency of the conventional RPA under investigation. A restricted RPA calculation dealing only with the collective degrees of freedom has already been advocated by Holtzwarth (5) on different grounds.

The electron gas hamiltonian may be written

$$H = \sum_{k,s} (k^2/2m)\, c_{k,s}^+ c_{k,s} + \sum_{q \neq 0} \sum_{k,k',s,s'} (2\pi e^2/q^2)$$
$$\times c_{k+q,s}^+ c_{k'-q,s'}^+ c_{k',s'} c_{k,s} \tag{2.1}$$

where $c_{k,s}$ is the annihilation operator for an electron of momentum k and spin s. Let us consider the following operators, wich we will use to create excited states,

$$A_{q;s,s'}^+ = N_q \sum_{k < k_{F'}|k+q| > k_F} c_{k+q,s}^+ c_{k,s'} , \tag{2.2}$$

where the normalization factor N_q is determined by the condition

$$< 0 | A_{q;s,s'}\, A_{q;s,s'}^+ | 0 > = 1 . \tag{2.3}$$

These operators are obviously related to the density operators

$$\rho_q = \sum_{i=1}^{N} exp\,(-i\,q.x_i) \tag{2.4}$$

which play an important role in electron gas theory (6), but we may also draw the inspiration for picking them up from an inspection of the potential term in eq. (2.1). We note that the vacuum of the operators $A_{q;s,s'}$ is the Hartree-Fock ground state $|0>$,

$$A_{q;s,s'} | 0 > = 0 . \tag{2.5}$$

The creation operators $A_{q;s,s'}^+$ generate states of nomentum q, when acting on $|0>$. Instead of the operators $A_{q;s,s'}^+$ we may consider

operators $A^+_{q;\,S;\,S_z}$ which generate states possessing definite spin quantum numbers S, S_z,

$$
\begin{aligned}
A^+_{q;\,1;\,0} &= 2^{-1/2}\left(A^+_{q;\,1/2,\,1/2} + A^+_{q;\,-1/2,\,-1/2}\right) \\
A^+_{q;\,1;\,1} &= A^+_{q;\,1/2,\,-1/2} \\
A^+_{q;\,1;\,-1} &= A^+_{q;\,-1/2,\,1/2} \\
A^+_{q;\,0;\,0} &= 2^{-1/2}\left(A^+_{q;\,1/2,\,1/2} - A^+_{q;\,-1/2,\,-1/2}\right).
\end{aligned}
\tag{2.6}
$$

However, for the sake of clarity, we will omit from now on the spin quantum numbers, but we will take spin into account when performing actual computations. We write, therefore, instead of eqs. (2.2) and (2.3),

$$
A^+_q = N_q \sum_{k\,<\,k_F,\ |k+q|\,>\,k_F} c^+_{k+q}\, c_k
\tag{2.2'}
$$

$$
<0\,|\,A_q\,A^+_q\,|\,0> = 1.
\tag{2.3'}
$$

We believe that the operators A_q are a good choice as boson operators because, if we consider quantities such us

$$
<0\,|\,A^2_q\,(A^+_q)^2\,|\,0> = 2 - N^2_q,
\tag{2.7}
$$

we find that the deviation from the ideal boson behaviour is very small, N^2_q being of the order of the inverse of the number of particles. If the A_q were true boson operators the right hand side of eq. (2.7) would be exactly 2.

It is now convenient to define the states

$$
\begin{aligned}
|q> &= A^+_q\,|0> \\
|q_1,\,q_2> &= A^+_{q_1}\,A^+_{q_2}\,|0>,\ \text{etc.}
\end{aligned}
\tag{2.8}
$$

and to introduce the hamiltonian

$$
\begin{aligned}
H_B &= E_{HF} + \sum_q \varepsilon_q\,A^+_q\,A_q \\
&+ \frac{1}{2}\sum_q g_q\left(A^+_q\,A^+_{-q} + A_{-q}\,A_q\right).
\end{aligned}
\tag{2.9}
$$

This hamiltonian is equivalent to H, in the sense that

$$
\begin{aligned}
&<0|H_B|q> = <0|H|q>, \\
&<q_1|H_B|q_2> = <q_1|H|q_2> \\
&<0|H_B|q_1, q_2> = <0|H|q_1, q_2>
\end{aligned}
\tag{2.10}
$$

provided

$$
\begin{aligned}
\varepsilon_q &= <q|H|q> - <0|H|0> \\
g_q &= <q, -q|H|0>.
\end{aligned}
\tag{2.1}
$$

In the next section we will give explicit expressions for these quantities. We remark that the operator H_B is a truncated Hamiltonian, appropriate only for the harmonic approximation. The full equivalence between H and H_B in the subspace spanned by the vectors $|0>, |q>, |q_1, q_2>, \ldots$, requires that anharmonic terms be included in eq. (2.9). We try to bring H_B to the diagonal form

$$
H_B = E_{HF} + E_c + \sum_q \omega_q \theta_q^+ \theta_q
\tag{2.12}
$$

by performing a cannonical transformation

$$
\begin{aligned}
&\theta_q = x_q A_q - y_q A_{-q}^+, \\
&[\theta_q, \theta_{q'}] = 0, \quad [\theta_q, \theta_{q'}^+] = \delta_{q, q'},
\end{aligned}
\tag{2.13}
$$

so that

$$
x_q^2 - y_q^2 = 1.
$$

We arrive finally at the eigenvalue equations

$$
\begin{aligned}
\varepsilon_q x_q + g_q y_q &= \omega_q x_q \\
g_q x_q + \varepsilon_q y_q &= -\omega_q y_q
\end{aligned}
\tag{2.14}
$$

which determine the excitation energy

$$
\omega_q = (\varepsilon_q^2 - g_q^2)^{1/2}.
\tag{2.15}
$$

The correlation energy is given by

$$E_c = \sum_q \frac{1}{2} (\omega_q - \varepsilon_q) \ . \tag{2.16}$$

However, this correlation energy refers only to collective correlations and not to intrinsic correlations. In order to evaluate intrinsic correlations, an intrinsic hamiltonian may be introcuded by an equation analogous to eq. (1.11), or better still, by the method of Villars (7), but this refinement does not seem necessary because the intrinsic correlations appear to be small. The numerical results which we report in the next section show that eq. (2.16) does not suffer from the defficiency of eq. (1.9).

We may observe, in passing, that eqs. (2.14) may also be obtained in the context of Hartree-Fock time-dependent theory. Indeed, eqs. (2.14) determine the time evolution of the nonstationary Slater determinant

$$| \Phi (t) > = \exp \left(\sum_q z_q (t) A_q^+ \right) | 0 >$$

where

$$z_q (t) = x_q \exp (-i \omega_q t) + y_{-q} \exp (i \omega_q t) \ .$$

Imaginary values of ω_q reveal, therefore, instabilities of the Hartree--Fock state.

3. NUMERICAL RESULTS

We present now the results of the numerical calculation. It is convenient to introduce the constant $\alpha = (4/9 \pi)^{1/3}$ and to specify the density of the electron gas through the mean square radius per electron in units of the Bohr radius, i. e., the parameter $r_s = e^2 m / \alpha k_F$, where k_F is the Fermi momentum. The final results may be expressed in terms of the following sums

$$n_q = N^{-1} \sum_{k \varepsilon D_q} 1 \tag{3.1}$$

$$t_q = (2 m / (N k_F^2)) \sum_{q \varepsilon D_q} ((k + q)^2 - k^2) / 2 m \tag{3.2}$$

$$u_k = -(4\pi e^2/V) \sum_{k_1 \varepsilon D_q} 1/(k - k_1)^2 \tag{3.3}$$

$$v_{1_q} = (2m/(Nk_F^2))(4\pi e^2/V) \sum_{k_1,\, k_2 \varepsilon D_q} 1/(k_1 - k_2)^2 \tag{3.4}$$

$$v_{2_q} = (2m/(Nk_F^2))(4\pi e^2/V) \sum_{-k_1,\, k_2 \varepsilon D_q} 1/(k_1 - k_2 - q)^2 \tag{3.5}$$

$$v_{3_q} = (2m/(Nk_F^2)) \sum_{k \varepsilon D_q} (u_{k+q} - u_k) \tag{3.6}$$

In these expressions, N is the total number of electrons, V is the normalization volume and D_q is the set of values of k such that $k < k_F, |k + q| > k_F$.

In terms of these quantities we may write down expressions for ε_q and g_q, but now we must take into account the spin quantum number S of the mode excited. Of course, S is either 0 or 1. We have

$$\varepsilon_{q;S} = (k_F^2/2m)\left((t_q + v_{3_q} - v_{1_q})/n_q \right. \tag{3.7}$$

$$\left. + (1-S)(16/3\pi)\,\alpha\, r_s\, k_F^2\, n_q/q^2\right) \tag{3.8}$$

$$g_{q;S} = (k_F^2/2m)\left(-v_{2_q} + (1-S)(16/3\pi)\,\alpha\, r_s\, k_F^2\, n_q/q^2\right)$$
$$\omega_{q;S} = (\varepsilon_{q;S}^2 - g_{q;S}^2)^{1/2} \tag{3.9}$$

We now observe that

$$v_{2_q} = v_{1_q} - v_{3_q}. \tag{3.10}$$

We have, indeed

$$\sum_{-k_1,\, k_2 \varepsilon D_q} 1/(k_1 - k_2 - q)^2$$

$$= \sum_{k_1 < k_F,\, k_2 \varepsilon D_q} 1/(k_1 - k_2 - q)^2$$

$$- \sum_{k_1 < k_F,\, |q - k_1| < k_F,\, k_2 \varepsilon D_q} 1/(k_1 - k_2 - q)^2$$

$$= \sum_{k_1 < k_F, \, k_2 \, \varepsilon \, D_q} 1 / (k_1 - k_2 - q)^2$$

$$- \sum_{|k_1' + q| < k_F, \, k_1' < k_F, \, k_2 \, \varepsilon \, D_q} 1 / (k_1' - k_2) \ .$$

We also have

$$\sideset{}{'}\sum_{k_1, \, k_2 \, \varepsilon \, D_q} 1 / (k_1 - k_2)^2$$

$$= \sum_{k_1 < k_F, \, k_2 \, \varepsilon \, D_q} 1 / (k_1 - k_2)^2$$

$$- \sum_{k_1 < k_F, \, |k_1 + q| < k_F, \, k_2 \, \varepsilon \, D_q} 1 / (k_1 - k_2)^2 \ .$$

Subtracting these equations we finally prove eq. (3.10), which shows that we need not compute v_{1_q} and v_{3_q} separately, but only v_{2_q}. Our final expressions may be be written, introducing the new variable $x = q / k_F$,

$$
\begin{aligned}
n_q &= \frac{3}{8} \ x \left(1 - \frac{1}{12} x^2 \right) && \text{if } x \leqslant 2 \\
&= \frac{1}{2} && \text{if } x > 2
\end{aligned}
\tag{3.11}
$$

$$t_q = \frac{1}{2} x^2 \ . \tag{3.12}$$

For x less than 2 we have computed v_{2_q} by reducing it to a double integral which has been evaluated by the Monte Carlo method. We have then fitted the numerical results by a polynomial in x^2.

For $x > 2$ the integrations were performed analytically. Our final result is

$$v_{2_q} = (3/2\,\pi)\,\alpha r_s\,(0.10327\,x^2 - 0.017215\,x^4 - 0.016558\,x^6$$

$$+ 0.029059\,x^8 - 0.017362\,x^{10} + 0.0011048\,x^{12} + 0.0031108\,x^{14}$$

$$- 0.0014083\,x^{16} + 0.00024849\,x^{18} - 0.000016165\,x^{20})\quad \textit{if}\quad x < 2$$

$$= (3/2\,\pi)\,\alpha\,r_s\left[\frac{11}{15} + \frac{1}{30}\,x^2 + (4/(3\,x))\left(\frac{1}{5}\,s_1^5 - s_1^4 + s_1^3\right)\right.$$

$$\left. \times 1n\,(2\,s_1/x) + (4/(3\,x))\left(\frac{1}{5}\,s_2^5 + s_2^4 + s_2^3\right)1n\,(2\,s_2/x)\right]\quad \textit{if}\quad x > 2 \tag{3.13}$$

where

$$s_1 = x/2 + 1\ ,$$

$$s_2 = x/2 - 1\ .$$

The correlation energy becomes finally

$$E_c = \sum_{S=0}^{1}\,(2S+1)\,\frac{3}{4}\int_0^\infty x^2\,(\omega_{q\,;\,S} - \varepsilon_{q\,;\,S})\,dx\ . \tag{3.14}$$

In fig. 1 we have plotted, as a function of r_s, the total value of E_c and the contributions to E_c from each S. We have also plotted, for comparison, the results of Carr et al (8). The accuracy of our simplified calculation is remarkable. We have also found that for $r_s > 9.6$ the Hartree-Fock ground state is unstable (imaginary values for $\omega_{q\,;\,S}$ for low q and $S = 1$). This indicates that for low densities the anharmonic terms become important and should be added to eq. (2.9). We also show in fig. 1, by the curve labeled «without exchange», the result of neglecting exchange terms, i. e, the result of setting $v_{1_q} = v_{2_q} = v_{3_q} = 0$. The value of E_c obtained in this way is an upperbound (9) to the ground state energy of Wentzel's model (10) (meson-pair theory), which does not include exchange. The values of E_c without exchange are lower (larger in absolute value) than the corresponding values of the correlation energy of Carr et al., in the range of r_s considered. This is so because Carr et al. take exchange
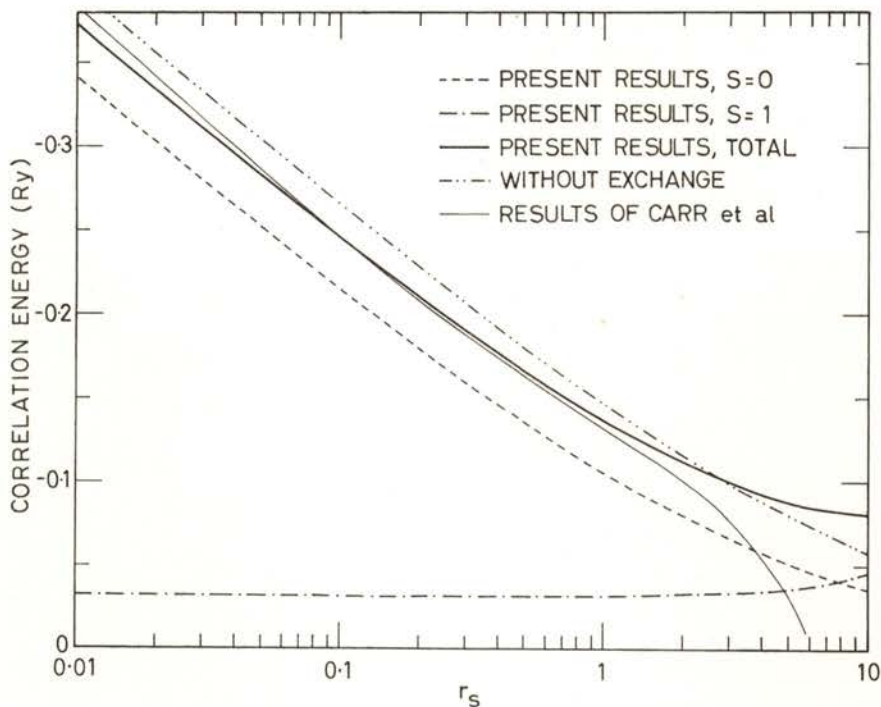
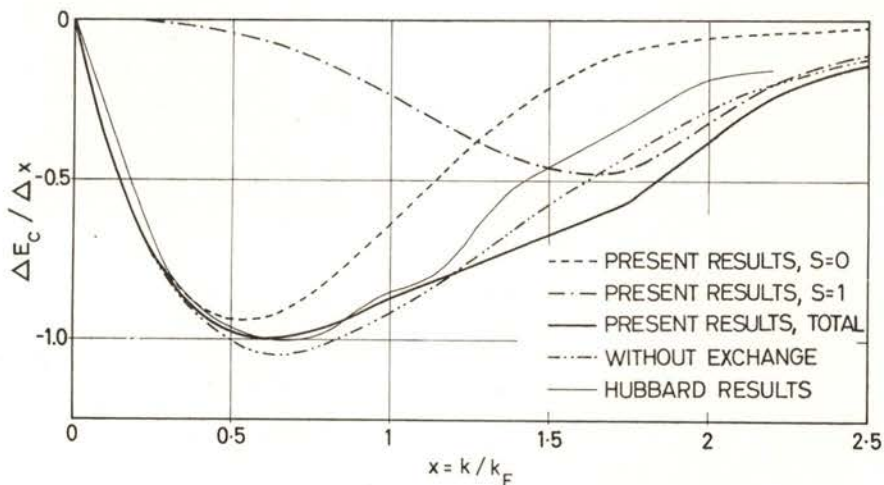Fig. 1 — The correlation energy as a function of the parameter r_s

Fig. 2 — The correlation energy per unit of x, for $r_s = 4$

into account and this contributes $+0.046$ Ry per electron to the correlation energy. At low densities, the neglect of exchange in our results provides an excellent approximation (11) to the ground state energy of Wentzel's hamiltonian.

In fig. 2 we plot, for $r_s = 4$, the partial contribution to E_c from each x, per unit of x, i. e., we plot the integrand of eq. (3.14). We also plot the partial contributions to the integrand of eq. (3.14) from each S. Comparision of our results with the results of Hubbard shows good agreement for x not very large. The curve labelled «without exchange» has been obtained by neglecting exchange terms, i. e., by setting $v_{1_q} = v_{2_q} = v_{3_q} = 0$ in our expressions. Exchange terms tend to reduce the absolute value of the correlation energy at low x. At high x the absolute value of the correlation energy is increased by the exchange terms, but then the anharmonic terms of the hamiltonian are probably important.

Finally we wish to emphasize that the present simplified calculation suggests a simple explanation for the discrepancy between eq. (1.9) arising from conventional RPA, and eq. (1.10), arising from partial summation of perturbation theory diagrams, namely, that the discrepancy is due to the violation of the RPA assumptions by noncollective RPA modes.

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