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Coupled clusters and Coulomb correlations

Document Version
Accepted author manuscript

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Published in:
Recent Progress in Many-Body Theories

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1. INTRODUCTION

In this paper I intend to give a summary of work carried out in the last few years on developments of the coupled-cluster formalism, and its application to infinite systems of either bosons or fermions. In particular I shall concentrate wholly on systems interacting via the two-body Coulomb force, and hence mainly, but not entirely, on problems involving the long-range behaviour of many-body systems. Much of this work on the one-component Bose and Fermi plasmas has been carried out in collaboration with K.H. Lührmann.

2. COUPLED-CLUSTER FORMALISM

I present first a brief outline of the main elements of the coupled-cluster formalism needed here. A full review of the formalism has recently been given,[1] although this deals almost exclusively with applications in nuclear physics, and hence largely with problems involving short-range correlations, rather than with the long-range correlations of the sort induced by the Coulomb force and which largely concern us here. The interested reader is directed to the article by Lührmann[2] for a formulation that perhaps best stresses its physical content, and to another article with the present author that sets the formalism firmly in the context of the one-component electron plasma.[3]

In terms of a suitable model, or uncorrelated, N-body wavefunction $|\Phi>$, the (usual linked-cluster) ansatz for the exact Coulomb-correlated N-body ground-state (g.s.) wavefunction $|\Psi>$,

$$|\Psi> = e^S|\Phi> , \qquad (1)$$

is made, and we consider $|\Psi>$ normalized to $|\Phi>$ by $<\Phi|\Psi> = 1$. I deal here with model Fermi states of Slater determinant form,

$$|\Phi_F> = a_{\nu_1}^\dagger \ldots a_{\nu_N}^\dagger |0> , \qquad (2)$$

with $|0>$ the vacuum state, and where the operators $a_{\nu_i}^\dagger$ are a set of fermion creation operators for the orthonormalized single-particle (s.p.) states $|\nu_i>$. For bosons, the antisymmetrized product of s.p. states is replaced by the (symmetric) single-state condensate,

$$|\Phi_B> = (N!)^{-\frac{1}{2}}(b_0^\dagger)^N|0> , \qquad (3)$$

where the operator $b_0^\dagger$ creates a boson in state o, and, more generally, the opera-

tors $b^+_{\alpha_i}$ create bosons in a complete orthonormal s.p. set $|\alpha_i\rangle$.

Although it is evidently possible to consider more general s.p. states, it is important for later discussions to realize that for all later results reported, I deal exclusively with plane-wave s.p. states. Thus $|\Phi_F\rangle$ represents the usual filled Fermi sea, and $|\Phi_B\rangle$ the usual completely occupied zero-momentum condensate: both isotropic, homogeneous states of zero total momentum. The correlation operator S is decomposed into n-body (n $\leq$ N) components,

$$S = \sum_{n=2}^{N} S_n , \qquad (4)$$

$$S_n = \begin{cases} (n!)^{-1} \sum\limits_{\rho_1 \ldots \rho_n} b^+_{\rho_1} \cdots b^+_{\rho_n} S_n(\rho_1 \ldots \rho_n)(N^{-\frac{1}{2}} b_0)^n; \text{ bosons} \\[2em] (n!)^{-2} \sum\limits_{\substack{\rho_1 \ldots \rho_n \\ \nu_1 \ldots \nu_n}} a^+_{\rho_1} \cdots a^+_{\rho_n} \langle\rho_1 \ldots \rho_n|S_n|\nu_1 \ldots \nu_n\rangle a_{\nu_n} \cdots a_{\nu_1}; \text{ fermions} \end{cases} \qquad (5)$$

The notation used in Eq.(5), and henceforth, reflects the linked-cluster aspect of the expansion, viz. s.p. labels ν_i indicate states normally occupied in $|\Phi\rangle$ (i.e. states inside the filled Fermi sea for fermions or the zero-momentum state, $\nu\equiv0$, for bosons); and s.p. labels ρ_i indicate normally unoccupied states. Where necessary later, s.p. labels α_i run over all s.p. states (i.e. a complete set). It is important to realize that the sum in Eq.(4) omits the term n=1 only as a consequence of our implied assumption that the exact g.s. wavefunction $|\Psi\rangle$ is also an eigenstate of total momentum (with eigenvalue zero).

Physically, S_n represents the true correlation operator for an n-body subsystem that remains after all the factorizable (or unlinked) correlations have been removed from the (complete) n-body subsystem amplitude operator Ψ_n, defined by its matrix elements,

$$\langle\alpha_1 \ldots \alpha_n|\Psi_n|\nu_1 \ldots \nu_n\rangle_A \equiv \langle\Phi|a^+_{\nu_1} \cdots a^+_{\nu_n} a_{\alpha_n} \cdots a_{\alpha_1}|\Psi\rangle, \text{ fermions}$$

$$\Psi_n(\alpha_1 \ldots \alpha_n) \equiv \langle\Phi|(N^{-\frac{1}{2}} b^+_0)^n b_{\alpha_n} \cdots b_{\alpha_1}|\Psi\rangle, \text{ bosons} \qquad (6)$$

where, for fermions, the subscript A on a ket state indicates an explicitly anti-symmetric state

$$|\nu_1 \ldots \nu_n\rangle_A \equiv a^+_{\nu_1} \cdots a^+_{\nu_n} |0\rangle .$$

Thus, for bosons as example, the 2- and 3-body subsystem amplitudes Ψ_2 and Ψ_3 can be expressed as,

$$\Psi_2(\alpha_1\alpha_2) = (N^{\frac{1}{2}}\delta_{\alpha_1,0})(N^{\frac{1}{2}}\delta_{\alpha_2,0}) + S_2(\alpha_1\alpha_2)$$

$$\Psi_3(\alpha_1\alpha_2\alpha_3) = (N^{\frac{1}{2}}\delta_{\alpha_1,0})(N^{\frac{1}{2}}\delta_{\alpha_2,0})(N^{\frac{1}{2}}\delta_{\alpha_3,0}) \qquad (7)$$

$$+ S_{123}[S_2(\alpha_1\alpha_2)(N^{\frac{1}{2}}\delta_{\alpha_3,0})] + S_3(\alpha_1\alpha_2\alpha_3),$$

in the thermodynamic limit $(N \rightarrow \infty$; volume $\Omega \rightarrow \infty$, $\rho = N/\Omega$ finite), and where S_{123} generates the sum of all terms obtained by cyclic permutation of the labels α_1, α_2 and α_3.

An equivalent physical description of S_n (for fermions) is that its matrix elements give the exact amplitudes that describe the excitation of n particle-hole pairs; where particles and holes refer respectively to states normally unoccupied and normally occupied (in the model wavefunction $|\Phi\rangle$). For bosons the role of the hole states is played by the condensate. It <u>seems</u> intuitively apparent that in order for our ansatz (1) to be useful, the physical system under consideration ought to share at least qualitatively the features built into the model state $|\Phi\rangle$. More explicitly we expect our choices $|\Phi_F\rangle$ and $|\Phi_B\rangle$ to have relevance respectively only to real fermion systems in states where some semblance of the sharp Fermi surface still remains, and to real Bose systems which contain a finite fraction of the particles in a zero-momentum condensate. This would seem to rule out from the outset for fermions, for example, an accurate description of "abnormal" or "super" phases, or indeed of anything but the usual "liquid" or "Fermi fluid" phase. Later, I give some indication that this intuitive feeling may well be false; or at least that the coupled-cluster formalism may be much more powerful than this too pessimistically narrow interpretation would seem to allow.

Formally, the g.s. coupled-cluster formalism now proceeds by decomposing the N-body Schrödinger equation

$$H|\Psi\rangle = E|\Psi\rangle \qquad (8)$$

into a coupled set of equations for the matrix elements of the correlation operators S_n. Formally this may be achieved by taking the overlap of Eq.(8) with the states $\langle\Phi|(a_{\nu_1}^{+}...a_{\nu_n}^{+}a_{\alpha_n}...a_{\alpha_1})$ for n = 0,1,...N, to get a set of coupled equations for the elements $\langle\Psi_n|\rangle$. Finally the amplitudes Ψ_n are decomposed in terms of the correlation amplitudes of the S_n, which has the effect of eliminating all macroscopic terms (<u>i.e.</u> those, like E, which are proportional to N) from the essentially microscopic subsystem equations. This wholly algebraic procedure results in a coupled set of equations for the elements of S_n, in which the ith equation for S_i is coupled to both S_{i+1} and S_{i+2} (as well as to all S_j with j<i), for a Hamiltonian H involving two-body potentials only. For the technical details of the derivation the reader is referred to Refs.[1-3]. Clearly, in order to be useful this exact coupled hierarchy needs to be truncated; and as an obvious initial step I discuss the so-called SUBn approximation scheme in which I set $S_i = 0$ for all i>n, and the remaining equations are treated as accurately as possible.

I now apply the coupled-cluster formalism to one-component Coulomb systems, stressing mainly the qualitative nature of the results in order more clearly to demonstrate the power of the formalism. To this end I spend more time on the mathematically much simpler boson equations, and indicate only more briefly their fermion counterparts.

3. APPLICATION TO ONE-COMPONENT COULOMB SYSTEMS

The Coulomb potential with a uniform, rigid and neutralizing background present is,

$$v(q) = \frac{4\pi e^2}{\Omega q^2}\left(1 - \delta_{\vec{q},0}\right) . \tag{9}$$

The density ρ may be expressed either in terms of the usual dimensionless coupling constant r_s, which is the average interparticle spacing in units of the Bohr radius a_0, or in terms of a (for bosons, fictitious) Fermi wavenumber k_F applicable to an unpolarized spin-$\frac{1}{2}$ system,

$$\rho = (4\pi r_s^3 a_0^3/3)^{-1} = k_F^3/3\pi^2 . \tag{10}$$

Henceforth, the g.s. energy per particle is expressed in Rydberg units by

$$E/N = \varepsilon(e^2/2a_0) , \tag{11}$$

and any dimensionless momentum variables that appear have been scaled against the Fermi momentum $\hbar k_F$, defined by Eq.(10).

3.1 Charged Bose system

For spin-zero bosons, the <u>exact</u> two-body equation for $S_2(q) \equiv S_2(\vec{q},-\vec{q})$ may readily be found by the method sketched in Sect.2:

$$\frac{\hbar^2 q^2}{m} S_2(q) + T_{RPA} + T_{CP} + T_{LAD} + \sum_{\vec{q}'} v(q')[2N^{\frac{1}{2}}S_3(\vec{q},\vec{q}',-\vec{q}-\vec{q}') + \tfrac{1}{2}NS_4(\vec{q},-\vec{q},\vec{q}',-\vec{q}')] = 0, \tag{12}$$

$$T_{RPA} = Nv(q)[1+S_2(q)]^2; \quad T_{CP} = -4\frac{E}{N}S_2(q); \quad T_{LAD} = \sum_{\vec{q}'} v(\vec{q}-\vec{q}')S_2(q'),$$

and where the g.s. energy per particle is given by,

$$E/N = \tfrac{1}{2}Nv(0) + \tfrac{1}{2}\sum_{\vec{q}} v(q)S_2(q) . \tag{13}$$

The SUB2 approximation is obtained from Eq.(12) by putting S_3 and S_4 to zero. The remaining first four terms in Eq.(12) represent respectively (i) the kinetic energy (KE) contribution, (ii) the terms that generate the ring or bubble diagrams of the random-phase approximation (RPA), (iii) the terms that generate the self-consistent (s.c.) energy insertions on the zero-momentum condensate lines, i.e. the s.c. condensate potential (CP), and (iv) the terms that scatter the two particles outside the condensate and hence generate the two-particle ladder (LAD) diagrams. Inserting the potential from Eq.(9) into the SUB2 equation gives, in dimensionless variables,

$$q^2 S_2(q) + 4\alpha r_s(3\pi q^2)^{-1}[1+S_2(q)]^2 - 2(\alpha r_s)^2\varepsilon S_2(q)$$

$$+ \frac{\alpha r_s}{\pi q} \int_0^\infty dq'q'\ln\left|\frac{q'+q}{q'-q}\right|S_2(q') = 0; \tag{14}$$

$$\varepsilon = 2(\pi\alpha r_s)^{-1}\int_0^\infty dq\, S_2(q), \tag{15}$$

where $\alpha \equiv (9\pi/4)^{-1/3}$.

Although Eqs.(14) and (15) are readily amenable to numerical solution, it is more instructive here to examine them in the high density $(r_s \to 0)$ and low density $(r_s \to \infty)$ limits. In the high density limit it is readily shown that to leading order for the energy only the KE and RPA terms contribute. The resulting quadratic equation is trivially solved to give

$$\epsilon \underset{r_s \to 0}{\longrightarrow} \epsilon_{RPA} = Q\, r_s^{-3/4}$$

$$Q = -2\pi^{-1}(6^{1/4})\int_0^\infty dx[1+x^4-x^2(x^4+2)^{1/2}] \approx -0.8031 ,$$

(16)

which is the exact result first obtained by Foldy.[4] It is not difficult to show that the next term in the high-density expansion is a constant,

$$\epsilon \underset{r_s \to 0}{\longrightarrow} Q\, r_s^{-3/4} + R ,$$

(17)

and that both the CP and LAD terms now contribute to R. I find,

$$R_{SUB2} = R_{CP} + R_{LAD}; \quad R_{CP} = 16/15\pi, \quad R_{LAD} = 32/45\pi .$$

(18)

By inspecting Eq.(12) and the equivalent equations for S_3 and S_4 it can however be shown that the coupling terms to S_3 and S_4 in the exact Eq.(12) also contribute to the constant R (although not to Q). I have also calculated the constant R given by the exact two-body Eq.(12), keeping the complete coupling to three- and four-body clusters. I find that, to this order, the 3-body correlation amplitude S_3 needed in Eq.(12) may be replaced by,

$$-N^{1/2}S_3(\vec{q}_1,\vec{q}_2,\vec{q}_3) \to [\omega(q_1)+\omega(q_2)+\omega(q_3)]^{-1}S_{123}[\{v(q_1)(1+S_2(q_1))$$
$$+ v(q_2)(1+S_2(q_2))\}S_2(q_3)],$$

(19)

for $\vec{q}_1+\vec{q}_2+\vec{q}_3 = 0$, and where the effective s.p. energy is,

$$\omega(q) = \hbar^2q^2/2m + Nv(q)(1+S_2(q));$$

(20)

and a similar replacement may be made for S_4 by examining the 4-body equation. Equations (12) and (13) then lead to

$$R = R_{SUB2} + R_3 + R_4 \approx 0.0280$$

(21)

where both the contributions R_3 and R_4 from the coupling terms to S_3 and S_4 in Eq.(12) are finite. The final result of Eq.(21) is exact, and an extremely tedious rearrangement of the integral expressions shows it to be in precise agreement with the first correct result reported, of Brueckner.[5] It is worth pointing out that, by contrast with most competing methods, each of the terms in Eqs.(18) and (21) is finite, and no cancellation of spurious logarithmic singularities occurs. This particular point highlights a more general advantage of the coupled-cluster formalism — namely that terms which tend to cancel each other are automatically grouped together.

Turning now to the more revealing low-density limit, naively one would not expect the SUB2 approximation to give any reasonable result at all in this strong-

coupling regime, since one imagines that the n-body clusters even with $n \gg 2$ are still very important. Indeed one believes the real Coulomb system to undergo a phase transition to a Wigner solid[6] in this limit, and the solid may be regarded as an archetypal system where the N-body correlations <u>dominate</u>. At any rate it is clear that the low-density Coulomb systems provide one of the most stringent tests for our formalism.

It is readily seen from Eqs.(14) and (15) that in the SUB2 approximation,

$$\varepsilon_{SUB2} \xrightarrow[r_s \to \infty]{} - A r_s^{-1} + B r_s^{-3/2} + O(r_s^2), \qquad (22)$$

where the KE term contributes only to the constant B in leading order. In this limit the terms RPA, CP and LAD are all necessary for a quantitative evaluation of the constant A, but they play distinctly different qualitative roles. Thus it is vital to keep the RPA terms to get the correct analytic behaviour because, as expected, these terms continue to be crucial for the long-range $(q \to 0)$ screening of the Coulomb potential. Similarly the CP plays a crucial role now in the short-range $(q \to \infty)$ limit. Whereas the inclusion of the LAD term quantitatively changes the constants A and B in Eq.(22), it may safely be omitted without changing the analytic form of Eq. (22). Dropping the LAD term from Eq.(14), I find

SUB2 - LAD approxn.: $A = (32/3\pi^2)^{1/3} \approx 1.03$; $B = 3^{1/2}\pi/8 \approx 0.68$. (23)

Use of the virial theorem verifies our expectation that the leading term in Eq.(22) is purely potential energy; and furthermore shows that the much more interesting second term is exactly one half each kinetic and potential energies — which at the very least is strongly reminiscent of simple harmonic motion and of the behaviour expected of a <u>solid</u>.

Indeed, as first pointed out by Wigner,[6] the energy of the system is minimised in this low density limit by the particles crystallizing into a regular periodic lattice, which leads to an electrostatic potential energy proportional to r_s^{-1}. Whereas in a fluid phase the particles are free to occupy the whole volume, which by the uncertainty principle leads to a kinetic energy proportional to r_s^{-2}, in the Wigner solid phase the particles are constrained to oscillate about the fixed lattice sites and hence to have a greater kinetic energy. Elementary considerations of simple harmonic motion lead to a kinetic energy proportional to $r_s^{-3/2}$. The <u>exact</u> expansion in the Wigner solid phase is a power series in $r_s^{-1/2}$ where the terms of order r_s^{-2} and higher are due to anharmonicities in the zero-point motion. Based on a b.c.c. lattice, Carr <u>et al.</u>[7] give,

$$\varepsilon_{exact} \xrightarrow[r_s \to \infty]{} - 1.792\, r_s^{-1} + 2.65\, r_s^{-3/2} - 0.73\, r_s^{-2} + \cdots . \qquad (24)$$

Clearly our approximation in Eqs.(22) and (23) has the correct analytic form for the energy of a solid, although the values of the coefficients are considerably under-estimated. What is more important however is that even the lowest SUB2 approximation in the coupled-cluster scheme gives a low-density energy which cannot possibly repre-

sent what is normally understood by a fluid phase, since the particles are definitely
not free to occupy the whole volume.

Thus it is clear that our intrinsically fluid-like and everywhere translationally-
invariant approach can provide a good description of both fluid and solid phases; and
we can understand the possibility of this by similar reasoning to that behind the
familiar "floating crystal model" of Feenberg.[8] On the other hand, we must still face
the fact that three- and more-body effects can only be treated in SUB2 approximation
in an average sense, and cannot possibly represent the detailed internal structure of
a lattice wavefunction. While I have presented explicit evidence that this is not a
severe limitation at least as far as the qualitative behaviour of the g.s. energy is
concerned (and probably also for matrix elements of other few-body operators), the
fact remains that for a charged Bose system in the low-density limit, the third and
higher order correlations are still very strong. Thus accurate values of the coeffi-
cients A and B cannot be expected. I note here that numerical calculations of the
complete SUB2 equation including the LAD term do not change this overall picture. In
fact our approximate value of A from Eq.(23) is lowered by about 20% by including the
LAD term, thereby increasing the discrepancy with the Wigner value. (I note also
however that an evaluation of the two-body radial distribution function within the
SUB2 approximation gives a positive-definite function at all densities only so long
as the LAD term is included.)

Finally I note that although the SUB2 approximation works superbly over the
entire density regime for the Bose Coulomb system, the g.s. energy is quantitatively
unsatisfactory in the low-density limit. It is clear that higher-order clusters must
be incorporated; but due to the relative simplicity of the Bose coupled-cluster equa-
tions this is quite practicable, as indeed I have already indicated in the high-
density limit.

3.2 Charged Fermi system

The SUB2 equations for fermions, although conceptually similar to those for
bosons, are mathematically vastly more complex due both to the many more terms re-
quired by antisymmetrization, and to the state- (i.e. momentum-) dependence induced
by the hole states inside the Fermi sea in comparison with the unique zero-momentum
condensate for bosons. In particular for fermions the matrix elements $S_2(\vec{k}_1, \vec{k}_2; \vec{q}) \equiv$
$\langle \vec{k}_1 + \vec{q}, \vec{k}_2 - \vec{q} | S_2 | \vec{k}_1, \vec{k}_2 \rangle$ depend not only on a momentum transfer $\vec{q}$ as for bosons but
also on the two hole momenta $\vec{k}_1$ and $\vec{k}_2$. The complete SUB2 equation for charged
Fermi systems has been discussed in detail,[3] and it is clear that a numerical solution
of this non-linear integral equation for a function of three 3-vectors, while perhaps
just feasible, is not to be undertaken lightly! Accordingly we have again examined
various limits and approximation schemes for handling the coupled-cluster Fermi equa-
tions, and I now briefly report on these.

In the high-density limit, the RPA again gives the leading contribution to the
correlation energy, ε_c, i.e. the g.s. energy relative to the (uncorrelated) Hartree-

Fock energy. In Ref.[3] the nonlinear integral equation for S_2 in RPA was solved exactly and in some detail, both confirming the well-known results of Gell-Mann and Brueckner,[9] and giving for the first time exact analytic forms for the four-point function S_2 and the once-integrated three-point particle-hole vertex function. The Tamm-Dancoff approximation (TDA) to the ring summation was also formulated, and the analogous exact solutions in TDA were also presented for the electron gas for the first time.

Turning to the intermediate-coupling ($1 \leq r_s \leq 5$) metallic-density regime, we no longer expect the RPA plus second-order exchange to be a good approximation, although it gives the first two terms in the high-density expansion for ε_c exactly. Thus, quite apart from ignoring (a) the simple exchange effects necessary to antisymmetrize RPA, we have ignored even in SUB2 approximation: (b) all of the combined particle-particle and hole-hole ladder terms, some at least of which are important for the correct short-range behaviour; (c) the generalized self-energy correction terms which self-consistently generate both the particle potential and, much more importantly the hole potential (which now for fermions plays the same crucial role as the CP for bosons); (d) classes of higher ring-exchange terms; and (e) a class of additional exchange terms which includes the particle-hole ladder terms. In order systematically to deal with these effects I have proposed and implemented a further approximation that enables us to study these terms much more readily.

Based on a comparison with Bose systems, the fermion equations should be much simpler if they could be "state-averaged"; and the basic approximation is thus to average over the initial hole momenta $\vec{k}_1$ and $\vec{k}_2$ in $S_2(\vec{k}_1,\vec{k}_2;\vec{q})$ but keeping the important exact property that final states $(\vec{k}_1+\vec{q})$, $(\vec{k}_2-\vec{q})$ lie outside the Fermi sea (i.e., the Pauli principle is exactly implemented). In this way the exact $S_2(\vec{k}_1,\vec{k}_2;\vec{q})$ is replaced by an averaged $\overline{S}_2(q)$, and the resulting coupled-cluster equation considered still then itself has to be state-averaged. Although the procedure for this latter step is not unique, this works to our advantage, for two reasons: (a) the averaging can be made on physically-motivated grounds rather than being imposed arbitrarily; and (b) since we know exact results for S_2 in at least one limit, namely the RPA and TDA results for $r_s \rightarrow 0$, the errors induced by the various averaging schemes can be checked. As an illustration: carrying out the above scheme in RPA leads to an equation for S_2 which involves only KE and RPA terms. After the replacement $S_2 \rightarrow \overline{S}_2$ has been made the only state-dependence left is in the KE term, which for fermions is proportional to $[|\vec{k}_1+\vec{q}|^2+|\vec{k}_2-\vec{q}|^2-k_1^2-k_2^2]S_2 \equiv eS_2$. As two obvious averaging schemes one could imagine (a) replacing $e \rightarrow <e>$; or (b) the intuitively and physically more appealing idea of first dividing through by e and then averaging the "energy denominator"; $e^{-1} \rightarrow <e^{-1}>$. I have shown that the former procedure leads precisely to the mean-spherical approximation (which Zabolitzky[10] discusses in this context, and which his state-independent, variational, Fermi hypernetted-chain (FHNC) formalism leads to in this $r_s \rightarrow 0$ limit), which gives an ε_c in error by 8.4% at $r_s \rightarrow 0$. The latter procedure on the other hand is exact at

$r_s \to 0$, and by comparison with the exact RPA results I show that it is for no density in error by more than 2%. There seems to be no reason why this result should not hold for all other terms in the Fermi SUB2 equation, which we may therefore now with confidence systematically include.

Based partly on experience with the Bose equations, our best coupled-cluster (CC) calculations to date, for ε_c in the metallic regime, include from the S_2 equation the following terms, all treated simultaneously and fully self-consistently: (i) KE; (ii) RPA; (iii) hole potential (HP); (iv) all particle-particle ladder (LAD) terms included in SUB2 and furthermore (motivated by experience with nuclear matter) a much broader class of generalized ladder terms obtained by taking into account part of the coupling terms to S_3 and S_4, and which involves replacing the bare potential by a self-consistent G-matrix (obtained from the full S_2 solution itself); (v) a class of particle-hole ladder terms called PHA in Ref.[3]; and (vi) exchange (EX) terms to keep the resulting S_2 explicitly antisymmetric. The results of this CC calculation are shown in the Table below, where for comparison I also show both the essentially exact (unpublished) results of Ceperley who used an approximate Green's function Monte Carlo (GFMC) method; and, as representatives of the best variational results, the FHNC results of both Zabolitzky[10] (FHNC-Z) and Lantto[11] (FHNC-L).

Table: The Fermi correlation energy ε_c for the unpolarized electron gas

r_s	ε_c(CC)	ε_c(GFMC)	ε_c(FHNC-Z)	ε_c(FHNC-L)
$\to 0$	$0.0622 \ \ell n \ r_s$	$(0.0622 \ \ell n \ r_s)$	$0.0570 \ \ell n \ r_s$	?
1	-0.123	-0.121	-0.114	-0.140
2	-0.0917	-0.0902	-0.0859	-0.098
3	-0.0751	...	-0.0710	-0.079
4	-0.0644	...	-0.0612	-0.067
5	-0.0568	-0.0563	-0.0541	-0.058

Turning finally to the low-density limit, the situation for fermions is much more favourable than for bosons since the Pauli principle very effectively hinders electrons from clustering in groups of more than two, thus forcing the higher correlations to be smaller. Although in the exact Wigner low-density limit the effects of quantum statistics vanish, with the fermion and boson solid both described by the same asymptotic expansion (24) (and the different statistics reflected only in differing terms which vanish exponentially with $r_s \to \infty$) this is by no means true in our translationally-invariant CC description. In the case of electron system, exchange terms do not vanish and the convergence of the CC hierarchy is thereby considerably improved from the Bose case. Thus for the analogue of the result (23) for bosons, I find $A \approx 1.58$ for electrons in a "state-averaged" RPA+HP scheme — which is in much better agreement with the Wigner solid value of 1.79.

4. FINAL REMARKS

I intend further to explore the low-density regime with the full SUB2 approximation for electrons since it provides a scheme that offers what is essentially the

first <u>unified</u> framework in which to calculate at <u>all</u> densities the g.s. properties (at least) of the charged quantum fluids/solids. Although I have stressed only g.s. energy calculations it is important to realise that recent extensions of the CC formalism permit calculations both of excited states and of the density matrices. For excited states, Emrich has given a very elegant formulation in which he derives a coupled set of eigenvalue equations for the energies and amplitudes of the excitations. As a first step I have applied this formalism in its lowest level of approximation to the electron plasma as $r_s \to 0$. As input this requires the exact g.s. (RPA) S_2 already found.[3] To this level of approximation I find the usual <u>plasmon</u> "bound-state" plus the one-particle-one-hole scattering continuum. Of particular interest at the next step will be the usefulness of the excited states to pin down further the low-density solid aspects of the g.s. calculations. Thus presumably the real electron system has plasmon excitations (with a finite energy gap at low momenta q) at high densities, and a phonon spectrum (with an acoustic branch linear in q at small q) characteristic of solids at low densities. It will be of great interest to see whether this behaviour is also seen in our calculations; and, if so, whether it can be used to obtain the critical density.

It is also intended further to examine the one- and two-body density matrices at metallic and low densities, since these can provide much more sensitive tests of various theories than the g.s. energy. For example, while the approximation RPA+EX gives quite good values for the g.s. energy at metallic densities, the density matrices can be badly wrong — even giving negative values for the two-body radial distribution function at small separations. All preliminary investigations indicate that the CC calculations also give extremely good Coulomb distribution functions.

Finally, work is also in progress to extend these results to such multi-component plasmas as the hydrogen plasma, simple metals, and the electron-hole droplets observed in various semiconductors (with a particular aim to study the excitonic phase).

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