Physica 108B (1981) 873-874
North-Holland Publishing Company

COUPLED CLUSTERS AND THE ELECTRON GAS AT METALLIC DENSITIES

R.F. Bishop and K.H. Lührmann

Department of Mathematics
University of Manchester Institute of Science and Technology
P.O. Box 88, Manchester M60 1QD, England

The coupled cluster formalism is applied to ground-state correlations in jellium. A state-averaging procedure which enables us to include essentially all of the important microscopic effects at metallic densities, is shown by comparison with exact RPA results to be accurate to about 1%. Our final results at metallic densities are also compared with recent exact stochastic simulations of the many-body Schrödinger equation and seen to be accurate to the same level. They probably therefore provide the currently best available microscopic description of this system.

The coupled-cluster formulation of quantum many-body theory has been discussed in some detail by the present authors [1], and applied to the problem of ground-state correlations in the one-component electron plasma. Attention was initially focussed on the high-density limit and the problem was completely solved in both the random phase approximation (RPA) and in the Tamm-Dancoff approximation (TDA). We report now on much more complete calculations appropriate to the metallic density regime.

The coupled cluster formalism exactly decomposes the N-body system into a set of mutually interacting n-body subsystems ($n = 1,\ldots,N$) by use of the familiar linked-cluster [or exp(S)] Ansatz acting with reference to some model (non-interacting) state, which we consistently take to be the usual filled Fermi sea appropriate to an unpolarized, spin-$\frac{1}{2}$, homogeneous system. The subsystems are hence described by a set of correlation operators S_n, whose matrix elements give the amplitudes for exciting n particle-hole pairs from the model state. The exact N-body Schrödinger equation for the ground state (g.s.) decomposes into a coupled set of N non-linear microscopic equations for these matrix elements, in which all macroscopic terms, proportional to N, are absent. The general structure of this set of equations is that the n^{th} equation in the hierarchy for S_n, is coupled, in the general case where the elementary Hamiltonian contains up to j-body forces, to all higher amplitudes S_{n+i} with $1 \leq i \leq j$ as well as to all lower S_m with $m < n$. In the present case we are interested only in $j=2$ Coulomb forces. In order to be useful this exact hierarchy of equations must be broken, and the so-called SUBn approximation does this by setting each S_i to zero for $i > n$. For translationally-invariant systems, $S_1 \equiv 0$ by momentum conservation, and we primarily concern ourselves therefore with the SUB2 approximation. For an infinite medium the SUB2 equations are non-linear integral equations in three momenta for the (antisymmetrized) matrix elements

$$S_2(\vec{k}_1,\vec{k}_2;\vec{q}) \equiv \langle\vec{k}_1+\vec{q},\vec{k}_2-\vec{q}|S_2|\vec{k}_1\vec{k}_2\rangle_A ,$$

where the "hole" states are labelled by momenta $\vec{k}_1$ and $\vec{k}_2$ inside the Fermi sphere, and where spin labels are suppressed for ease.

We stress again that the basic SUB2 approximation is exact apart from neglecting interactions with higher-order subsystems. Otherwise all two-body effects are included, and it is hence no surprise that the equations are complex. As drastic sub-approximations to itself, the SUB2 approximation contains such other familiar approximations as RPA and TDA; the Bethe-Goldstone equation which sums the two-particle ladder diagrams, and more generally the whole of (lowest-order) Brueckner theory; and the Galitskii approximation which represents the ladder approximation to the Bethe-Salpeter equation.

In the high-density limit (i.e., the weak-coupling limit $r_s \to 0$, in terms of the dimensionless coupling constant r_s, which is the average interparticle spacing in units of the Bohr radius), the RPA gives the leading contribution to the correlation energy ε_c, i.e., the g.s. energy per particle relative to the uncorrelated (Hartree-) Fock energy (and with all energies expressed in Rydberg units). In Ref. [1] the nonlinear integral equation for S_2 in RPA was solved exactly and in some detail.

In the intermediate-coupling regime ($1 < r_s < 5$) of metallic densities we no longer expect RPA to suffice. Thus, quite apart from ignoring (i) the simple exchange terms needed to antisymmetrize RPA, we have neglected even in SUB2 approximation: (ii) all combined particle-particle and hole-hole ladder terms, some at least of which are important for correct short-range behaviour; (iii) the self-energy correction terms which self-consistently generate both the particle potential and the more important hole potential; (iv) classes of higher ring-exchange terms to preserve overall antisymmetry; and (v) other exchange terms which include the particle-hole ladders. In order systematically to go beyond RPA and to include these effects we have developed a further "state-averaging" approximation, motivated by the analogy with the mathematically

0378-4363/81/0000-0000/$02.50

much simpler Bose equations. Our basic approximation is to average inside the Fermi sea over the hole momenta $\vec{k}_1$ and $\vec{k}_2$ in $S_2(\vec{k}_1,\vec{k}_2;\vec{q})$ but to preserve the Pauli principle by insisting at the same time that the particle momenta $(\vec{k}_1+\vec{q}),(\vec{k}_2-\vec{q})$ lie outside the Fermi sea. The exact $S_2(\vec{k}_1,\vec{k}_2;\vec{q})$ is thereby replaced by an averaged $\bar{S}_2(q)$, and the resulting coupled-cluster equation must itself still be suitably state-averaged. Although this latter step is not unique we may use this to our advantage, since the averaging may be made on physically-motivated grounds. Further, since we know exact results for S_2 in at least one limit, namely the RPA and TDA results for $r_s \to 0$, the errors induced by the averaging procedures may be checked and controlled. As a simple illustration we imagine putting this cheme into effect for RPA, which comprises an equation for S_2 which involves only the kinetic energy (KE) and RPA terms [1]. After the replacement $S_2 \to \bar{S}_2$, the only state-dependence is in the KE term which takes the familiar form of being 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 either (i) replacing $e \to \langle e\rangle$; or (ii) the intuitively and physically more appealing replacement $e^{-1} \to \langle e^{-1}\rangle$ after dividing through by e first; i.e. averaging the two-body propagator or "energy denominator". We show that the former procedure leads precisely to the "mean spherical approximation" discussed by Zabolitzky [2] in this content, and which arises in his state-independent, variational, Fermi hypernetted chain (FHNC) formalism in this $r_s \to 0$ limit. Whereas this approximation is in error for ε_c (by comparison with exact results) by 8.4% at $r_s \to 0$, we show the latter procedure to be exact at $r_s \to 0$ and to give better than 2% accuracy for all densities. Further, there is no reason to expect markedly worse accuracy for all other terms in the Fermi SUB2 equations.

Our most complete results for metallic densities include the completely integrated and self-consistent effects of the terms which by themselves generate: (i) RPA and its exact long-range screening effects; (ii) the extra exchange effects to preserve antisymmetry; (iii) the self-consistent particle-particle ladders (LAD) that describe two-particle scattering within the many-body medium and which describe the exact short-range limiting behaviour; (iv) a class of particle-hole ladders; and (v) the self-consistent hole potential. Particular attention is paid to the important effects caused by the interference at intermediate separations of the long-range RPA and short-range LAD effects; and this necessitates even going beyond SUB2 to include a much broader class of generalized ladder terms from incorporating part of the coupling to S_3 and S_4, and which involves replacing the bare Coulomb potential in other SUB2 terms by a self-consistent G-matrix (obtained from the full S_2 solution itself). We also argue that all other SUB2 terms either cancel among themselves, or are negligibly small at metallic densities.

The results of this coupled cluster (CC) calculation are shown in Table I, and are compared both with the Green's function Monte Carlo (GFMC) results [3] which give an essentially exact stochastic simulation of the many-body Schrödinger equation, and with the FHNC results of Zabolitzky [2] as one of the best variational results available. Our accuracy seems to be of the order of 1% in the metallic regime; and it seems fair to say that our CC method provides what is probably now the best microscopic description of the electron gas at these densities.

Table I: Correlation energy of unpolarized jellium

r_s	ε_c(CC)	ε_c(GFMC)	ε_c(FHNC)
$\to$ 0	0.0622ℓn r_s	(0.0622ℓn r_s)	0.0570ℓn r_s
1	-0.123	-0.121	-0.114
2	-0.0917	-0.0902	-0.0859
3	-0.0751	...	-0.0710
4	-0.0644	...	-0.0612
5	-0.0568	-0.0563	-0.0541

REFERENCES

[1] Bishop, R.F. and Lührmann, K.H., Phys.Rev. B17 (1978) 3757.

[2] Zabolitzky, J.G., Phys.Rev. B22 (1980) 2353.

[3] Ceperley, D.M. and Alder, B.J. (unpublished).