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PAIRING CORRELATIONS, COMPOSITE PAIRS, COUPLED CLUSTERS AND ALL THAT

by

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Abstract: The coupled cluster [or $\exp(S)$] formulation of quantum many-body theory is first extensively reviewed. It is then applied to the general problem of pairing correlations within a many-fermion system. The method is illustrated by restricting ourselves to the exact calculations that can be performed within the various generalized ladder approximations. It is shown how the formalism provides an efficient and unified framework in which to describe all aspects of pairing at the same level of approximation. Possible extensions to deal with composite clusters of more than two particles and to incorporate the effects of the collective excitations, are sketched.

I. Introduction

Many-body calculations on the scattering and binding properties of constituent pairs of fermions imbedded in a large, typically infinite, background of identical particles, have historically played a crucial role both in understanding the observed properties of many systems of condensed matter [1], and also for developing and understanding the various formulations of many-body theory itself. Furthermore, bound pairs within the many-body medium serve as the simplest example of the more general problem of the existence and nature of bound clusters within many-body systems, and the resulting effects of such clustering on the macroscopic properties of these systems.

To discuss pairing microscopically, the key element in one type of formulation is some sort of effective two-body scattering amplitude (G-matrix, T-matrix, etc.). Although not open to direct physical observation, such a pair amplitude is then usually used in one of two ways; namely either as an effective link with thermodynamic and average single-particle behaviour [2], or in microscopic perturbation theories as a new lowest-order element in a useful if not vital rearrangement of the perturbation series [3]. Probably the best known and most successful application of such ideas was the identification of Cooper pairs [4] as bound electron pairs within a many-electron system, and their responsibility for the phenomenon of superconductivity.

Pairing correlations within a many-body system have most frequently been discussed within the context of many-body perturbation theory for the (non-degenerate) ground-state energy. Such calculations have largely fallen into two main types. On the one hand there are those calculations using the time-independent formalism, which can conveniently be represented via the linked-cluster expansion of Goldstone [3] in the diagrammatic language of (time-ordered) Goldstone diagrams. On the other hand there are the calculations which employ time-dependent perturbation theory, which usually start from the Green's function formalism of Galitskii and Migdal [5], and which can in turn be formulated in the diagrammatic language of (non-time-ordered) Feynman diagrams. Relations between the two approaches have been discussed by the present author [6], particularly at the level of their (different) respective ladder approximations discussed more fully below.

From the physical viewpoint, the existence of bound or composite clusters of fermions within a many-fermion system is of considerable importance, since under suitable conditions any such even-numbered complexes (or composite bosons) may condense, leading to a possible phase transition in the system. In this context it is useful to recall the classification of composite bosons by Kohn and Sherrington [7] into two types. Thus, Type I comprise the complexes of an even number of real fermions (particles) and/or an even number of their corresponding holes; and Type II comprise the bound complexes of particle-hole pairs, more generally known as collective or giant excitations. Type I composite bosons are exemplified by ^4He atoms or Cooper pairs; while phonons, plasmons and the giant resonances in atomic nuclei are examples of Type II. Kohn and Sherrington particularly stressed the important point that when a system of Type I bosons condenses the resulting macro-state exhibits ordering in momentum space or off-diagonal long-range order (ODLRO) in coordinate space, which in turn leads to a superfluid-like phase. Conversely, the condensation of Type II bosons does not lead to ODLRO, but rather there is a change of long-range order in coordinate space (diagonal long-range order). Typical examples are the condensation of the Type I Cooper pairs into the superconducting phase; and the condensation of Type II excitons in the so-called excitonic phase of a photoexcited semiconductor, in which the excited electron-hole droplets become unstable against the formation of a coherent condensate of bound electron-hole pairs (or excitons). Another, perhaps less familiar, example of Type II condensation occurs in a crystal when a macroscopic number of phonons undergo Bose condensation into a single mode. This leads to a distortive phase transition of the crystal and the appearance of a superlattice.

In this work we start from the premise that one of the most interesting general problems in modern quantum many-body theory is the interplay between, and the mutual effects on each other of, the many-body collective excitations and other collective aspects of the system's behaviour on the one hand, with the low-lying single-particle, two-particle and few-particle excitations on the other hand. In the above language, one aspect of this problem is now cast as the interplay between the two types of composite bosons that may co-exist in the many-fermion system. Since it is also generally true that long-range interactions tend to accentuate the collective excitations, whereas

Short-range interactions tend to accentuate the few-body excitations, the general problem can also be interpreted in terms of the interplay between the long- and short-range correlations, both of which seem to be present to a comparable degree in such real systems of interest as nuclear matter and liquid ^3He .

One of the main aims of the work of which the present paper forms an introductory part, is to imbed the general problem just outlined in a many-body formalism which is both powerful and wide enough to encompass all aspects of it, and which we hope to demonstrate is uniquely equipped to provide practical solutions. The proposed formalism is the $\exp(S)$ method as it was originally called or, to give it its more modern name, the coupled cluster formalism (CCF) of Coester and Kümmel [8]. In the present work we focus initial attention on Type I pairing by formulating the generalised particle-particle and/or hole-hole "ladders" within the CCF. In later work we intend to incorporate also all aspects of particle-hole pairing (both the particle-hole "bubbles" or "ring diagram" terms and the particle-hole "ladders"), self-consistent self-energy effects for both the particles and the holes, exchange (antisymmetry) and other effects outlined below. The philosophy of the present work is thus complementary to that already forming the basis of a series of articles by the present author and his co-author [9-11]. There, we addressed essentially the same problems but initial attention was focussed in the first paper [9] (hereafter referred to as I) on Type II pairing by first formulating within the CCF the generalised particle-hole "bubble" or "ring" terms. These terms are of particular importance for example to the electron correlations in the one-component Coulomb plasma (or "electron gas"), and are responsible for the plasmon modes. In a subsequent paper [10], the full power of the CCF was then brought to bear on the ground-state (g.s.) correlations in the one-component Coulomb plasma at low and metallic densities with remarkable success. In fact, by comparison with the essentially exact Green's function Monte Carlo results for this system, our results over the entire metallic density range were seen to be accurate to the 1% level and gave what was probably the best available microscopic description of this system. The present paper should now be viewed as analogous for particle-particle and hole-hole ladder terms to what was done in I for the particle-hole bubble terms.

In Section 2 we give an essentially heuristic formulation of the g.s. CCF, referring the reader to I for details. The extension of the CCF to excited states (e.s.) given by Emrich [12] is then sketched in Section 3. A comparison and further discussion of the g.s. and e.s. CCF methods is given in Section 4. In Section 5 we then discuss the formulation of (Type II) pairing correlations and composite pairs within the CCF and outline the exact analytic results obtained for a particular model interaction of interest. Finally we discuss in Section 6 what can be concluded from these preliminary investigations, and allude to future extensions of the work.

2. Ground-State Coupled Cluster Formalism

We consider a system of N identical fermions whose mechanics is governed by the nonrelativistic Schrödinger equation with a hamiltonian consisting of kinetic energies and two-body potentials V ,

$$H = \sum_{\alpha} \epsilon_{\alpha} a_{\alpha}^{\dagger} a_{\alpha} + \frac{1}{(2!)^2} \sum_{\alpha\beta\gamma\delta} \langle \alpha\beta | V | \gamma\delta \rangle_A a_{\alpha}^{\dagger} a_{\beta}^{\dagger} a_{\delta} a_{\gamma}, \quad (1)$$

where the operators a_{α}^{\dagger} are a set of fermion creation operators for the complete and orthonormal single-particle (s.p.) basis states $|\alpha\rangle = a_{\alpha}^{\dagger}|0\rangle$, with $|0\rangle$ the vacuum state. The quantities ϵ_{α} represent the s.p. kinetic energies, and the notation

$$|\alpha_1 \dots \alpha_n\rangle = |\alpha_1\rangle \dots |\alpha_n\rangle$$

has been introduced for a direct product state. Furthermore, the subscript A on the ket state denotes explicit antisymmetrization (without normalization), namely

$$\begin{aligned} |\alpha_1 \dots \alpha_n\rangle_A &= \sum_{P\{\alpha\}} (-1)^P |\alpha_1 \dots \alpha_n\rangle \\ &= a_{\alpha_1}^{\dagger} \dots a_{\alpha_n}^{\dagger} |0\rangle, \end{aligned} \quad (2)$$

where the sum extends over all $(n!)$ permutations of the indices $\alpha_1 \dots \alpha_n$ and P_{α} is the signature of the permutation.

The usual starting-point for the g.s. CCF is a formally exact decomposition of the exact many-body g.s. Schrödinger equation,

$$H|\psi\rangle = E|\psi\rangle \quad (3)$$

in terms of a set of nonlinear coupled equations for the so-called correlation amplitudes. The formalism has already been discussed in some detail in I. In terms of a suitable model, or uncorrelated, N -fermion normalized wavefunction $|\phi\rangle$, the (usual linked cluster) CCF ansatz for the exact, correlated, N -fermion g.s. wavefunction $|\psi\rangle$ is made,

$$|\psi\rangle = e^S |\phi\rangle; \quad S = \sum_1^N S_n, \quad (4)$$

and we suppose only that $|\phi\rangle$ is such that it has a non-zero overlap with $|\psi\rangle$, and in particular we consider $|\psi\rangle$ normalised to $|\phi\rangle$ by $\langle\phi|\psi\rangle = 1$. Although it is quite possible to start from more complicated model states, we deal for present purposes only with those of a single Slater determinant (or "filled Fermi sea") form,

$$|\phi\rangle = a_{\nu_1}^{\dagger} \dots a_{\nu_N}^{\dagger} |0\rangle. \quad (5)$$

Henceforth we use the standard notation that s.p. labels ν_i indicate states "normally occupied" in $|\phi\rangle$ and which hence correspond in the usual terminology with "hole states" when vacated; s.p. labels ρ_j indicate states outside the Fermi sea (i.e., "normally unoccupied" by reference to $|\phi\rangle$, or "particle states" free to be occupied), and s.p. labels α_i (and β, γ, δ) run over all states.

In an introductory work such as this, it is perhaps useful to give a heuristic and pedagogical interpretation of the particular exponential form (4), since this is absolutely central to the whole CCF approach. For such non-degenerate ground states considered here as those of closed-shell atoms, for example, it seems obvious that an important part of the electronic wavefunction is the Slater determinant $|\phi\rangle$ of occupied states. The underlying physical picture here is of course the extreme simplification of each electron moving independently in a potential well produced by the nucleus and the averaged motion of the other electrons, which themselves move independently except for the restrictions imposed by the Pauli principle. Due to the Pauli principle each electron is in a different

s.p. eigenstate (or "orbital") of this mean potential, and for the N-body g.s. in this extreme picture, we envisage the N lowest s.p. states being filled from below, as indicated in Fig.1(a), up to some Fermi level of energy ϵ_F , which is just the state $|\phi\rangle$. It

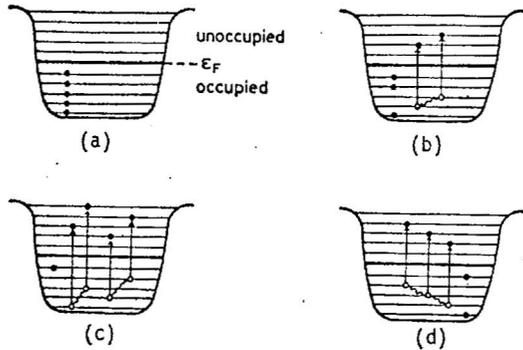


Figure 1: Schematic representations of (a) the filled Fermi sea state $|\phi\rangle$ and (b) a correlated pair, (c) two independent correlated pairs, and (d) a correlated triplet, excited out of it.

is of course precisely this picture which forms the basis of the well-known and successful Hartree-Fock theory.

But of course this picture of the filled Fermi sea is still far from complete, since the particles will in general mutually interact and hence do not move independently from each other. Having already built the statistical correlations into $|\phi\rangle$, we now attempt to correct systematically for these extra *dynamical correlations*. The first correction one may imagine is from two particles mutually interacting, which thereby lift themselves out of the Fermi sea into previously unoccupied orbitals, as illustrated in Fig.1(b). This process is described by some operator S_2 which acts on the wavefunction $|\phi\rangle$ to produce the wavefunction $S_2|\phi\rangle$, which describes two particles outside the Fermi sea (and consequently two holes inside it), and all remaining $(N-2)$ particles in their previous orbitals. Of course, it may also transpire that two pairs of particles do this *completely independently*, as illustrated in Fig.1(c). This process is clearly described by applying the operator S_2 twice, but with the proviso that we must include a statistical weighting factor (or multiplicity) of $(2!)^{-1}$ to avoid counting the pairs twice. This process of independent pair excitation out of the Fermi sea may be continued to obtain a contribution $(m!)^{-1} S_2^m |\phi\rangle$ for the amplitude describing the simultaneous excitation of m independent pairs. We thus get the total amplitude for the excitation of all possible numbers (including zero) of independent pairs as

$$\sum_0^{\infty} \frac{1}{m!} S_2^m |\phi\rangle = \exp(S_2) |\phi\rangle.$$

Continuing in this way, we next imagine the simultaneous excitation of a correlated triplet of particles, as in Fig.1(d), which we describe by a contribution $S_3|\phi\rangle$ to the total exact wavefunction $|\psi\rangle$. Similarly there will be a contribution $(n!)^{-1} S_3^n |\phi\rangle$ from the simultaneous excitation of n independent, correlated triplets. Next, and most importantly, we can also imagine the simultaneous excitation from the Fermi sea of m pairs and n triplets, all indepen-

dently of each other, with an amplitude $(m!n!)^{-1} S_2^m S_3^n |\phi\rangle$. Here it is crucial to realise that the ordering of the product of operators S_2 and S_3 is immaterial, since as a consequence of the independence of the processes they describe, the operators commute. Summing over all possible values of m and n then leads to the amplitude $\exp(S_2 + S_3) |\phi\rangle$ to include the total effect of all pair and triplet excitations. Proceeding in this way with the excitation of clusters of 4, 5, ... N particles we arrive at a wavefunction $\exp(S_2 + S_3 + \dots + S_N) |\phi\rangle$.

And yet, even this is not quite the end of the story. It may still occur that during the interaction of any subset of particles only one of them is finally lifted out of the Fermi sea, whereas the others fall back inside. Any number of single particles may also thus be independently promoted out of the Fermi sea. As before one is led to describe this process by an operator $\exp(S_1) |\phi\rangle$, where S_1 acts on the state $|\phi\rangle$ to produce a single "particle-hole" excitation on top of it. It is of interest to note that this particular case has a special interpretation provided by the well-known Thouless theorem which states that the most general determinantal wavefunction $|\phi'\rangle$ not orthogonal to a given Slater determinant $|\phi\rangle$ has the form $|\phi'\rangle = \exp(S_1) |\phi\rangle$ for some suitable choice of one-body operator S_1 . In other words, the effect of allowing single particles to be independently elevated above the Fermi sea is equivalent to changing the s.p. orbitals or "shell-model basis states" that make up the Slater determinant. One may even think of choosing the "best orbitals" by a criterion which expresses that $|\phi\rangle$ should be as close as possible to the exact $|\psi\rangle$. If we choose for example to maximise the overlap integral $|\langle\phi|\psi\rangle|$, this fairly readily leads to the choice $S_1 = 0$. Furthermore, if higher correlations are also ignored (by setting $S_2 = S_3 = \dots = 0$), this "maximum overlap" condition for the s.p. orbitals becomes equivalent to the Hartree-Fock theory, although more generally the correlations induced by the operators S_n with $n > 1$ also influence the optimal s.p. basis thus defined. This discussion has some real bearing on later approximation schemes. Thus in general it is desirable to make $|\langle\phi|\psi\rangle|$ large, or what is the same, to make S small in some ill-defined but intuitively obvious sense. Although the choice of $|\phi\rangle$ may be strictly irrelevant if one includes *all* higher correlations induced by the operators S_n with $n = 2, 3, \dots, N$, this is not true when one approximates. Clearly, the better is the choice $|\phi\rangle$, the better is likely to be a low order approximation in terms of the operators S_n .

In any case we have obtained the natural exact decomposition of the N-fermion wavefunction of Eq.(5), together with a physical interpretation of both the exponential form and the individual operators S_n . From the discussion it is clear that the operators S_n only have matrix elements between n-particle and n-hole s.p. states, and hence have the form,

$$S_n = \frac{1}{(n!)^2} \sum_{\substack{\rho_1 \dots \rho_n \\ \nu_1 \dots \nu_n}} a_{\rho_1}^+ \dots a_{\rho_n}^+ a_{\nu_1} \dots a_{\nu_n} \langle \rho_1 \dots \rho_n | S_n | \nu_1 \dots \nu_n \rangle A \quad (6)$$

Apart from using the exponential form of Eq.(4) as its basis, the other most fundamental idea of the CCF is to compute the operators S_n , or in practice their matrix elements, directly. In this it fundamentally differs from such alternate methods as, for example, the configuration-interaction (CI) method and,

to a lesser degree, the perturbation-theoretic methods. The former differs, and ultimately suffers, by using combinations of clusters instead of the clusters described by the operators S_n themselves, with the result that numerical instabilities arise for large particle numbers N . The latter method depends by contrast much more strongly on the smallness of some effective coupling constant than does the CCF.

To exploit fully the concepts built into the CCF, one further technical trick is needed to avoid the mixing of "small" and "large" terms that otherwise would so easily lead to numerical instabilities (of the sort alluded to above in connection with the CI method) even in exact calculations, and disastrously wrong results in approximate calculations. We attempt now to describe the physical ideas behind this important point. As N becomes large, the energy E asymptotically scales as N^α , for some positive index α (e.g. $\alpha = 1$ for homogenous systems to make E an extensive variable; $\alpha = 2/3$ for atoms, as given by Thomas-Fermi theory). This produces terms that scale as N^α in the g.s. Schrödinger equation (3) -- these are the "large" terms above. But there will also be other "microscopic" (or "small") terms which are practically independent of N . That this must be so can be intuited from the fact that for most reasonable interaction hamiltonians, a given particle will typically interact with only a few (i.e., a microscopic number of) immediate neighbours at a time. (Admittedly the picture we have in mind here does depend on the bulk phase of the system insofar as it seems more appropriate, say, to a fluid than to a solid phase). Thus, although summing up all energy contributions from all interacting clusters (in the sense described by the correlation operators, S_n) must yield a contribution of order N^α , the dynamics of each individual cluster is governed in the main by the interactions with only relatively few others -- and hence in the equations of motion this must show up as a "microscopic" effect.

The formal trick already mentioned that automatically performs this separation of large and small terms or, equivalently, removes the "unlinked terms", is to write the Schrödinger equation (3) in the equivalent CCF form

$$e^{-S}He^S|\phi\rangle = E|\phi\rangle. \quad (7)$$

The operator product on the left-hand side of Eq.(7) has the well-known expansion in powers of S ,

$$e^{-S}He^S = H + [H, S] + \dots + \frac{1}{n!} [\dots [H, S], S] \dots, S] + \dots, \quad (8)$$

involving the repeated commutators of H once with S an arbitrary number of times. For a given hamiltonian containing, say, the sum of up to m -body potentials, it is trivial to see that the otherwise infinite expansion (8) actually terminates at the term involving at most $2m$ S -operators. When the S -operator is in turn expanded into its n -body pieces S_n as in Eq.(4), the mutual commutativity of these pieces then immediately implies that all remaining terms are "linked" (to the hamiltonian) and therefore microscopic, with the exception only of those terms that contribute to the energy E itself to yield equality with the right-hand side of Eq.(7).

The CCF equations for the g.s. that one actually solves are now readily found by projecting Eq.(7) onto either the model state $|\phi\rangle$ or onto those n -particle/ n -hole states,

$$|\phi_n(\rho, \nu)\rangle \equiv a_{\rho_1}^+ \dots a_{\rho_n}^+ a_{\nu_1} \dots a_{\nu_n} |\phi\rangle, \quad (9)$$

built on it, with $n \leq N$. The states $|\phi\rangle$ and $|\phi_n\rangle$ clearly span the entire Hilbert space when n runs over 1 to N and when the labels ρ_i and ν_i in Eq.(9) run over the entire s.p. basis for particles and holes respectively. Thus the resulting equations,

$$\langle\phi|e^{-S}He^S|\phi\rangle = E; \quad (10a)$$

$$\langle\phi_n(\rho, \nu)|e^{-S}He^S|\phi\rangle = 0; \quad n = 1, \dots, N, \quad (10b)$$

which are just the g.s. coupled cluster equations, are fully equivalent to (and just a cluster decomposition of) the g.s. N -fermion Schrödinger equation. Further evaluation of Eqs. (10) is straightforward although algebraically tedious. It has been discussed in some detail in I, and the resulting equations for $n = 1$ and 2 have been explicitly derived.

The N equations (10b) now represent a *truly microscopic* decomposition of the g.s. Schrödinger equation into a set of coupled equations which describe the dynamics of the n -body clusters for $n = 1, \dots, N$, in which the energy E and other macroscopic terms never appear. The equations are *intrinsically nonlinear* as we have seen, and for the hamiltonian of Eq.(1) with pairwise interactions only, this nonlinearity is expressed via powers of the matrix elements of the operators S_i no higher than the fourth. Also, the structure of the n^{th} equation (for matrix elements of S_n) is that it is coupled to the other m^{th} equations for all $m \leq n+2$. By formally *iterating* these equations in powers of the interaction potential, one may immediately regain the individual terms of the time-independent perturbation theory approach expressed in terms of the linked-cluster expansion of Goldstone [3]. We stress however that it is *never necessary* for the actual solution of our equations (10), and indeed the process may well diverge in practice. Expressed differently, what the CCF achieves in this way is a rather natural grouping of perturbation-theoretic terms (or Goldstone diagrams). While conceptually very simple, as we have been at pains here to show, it is no surprise that even in very low order cluster equations (truncated as discussed below), the number of equivalent Goldstone diagrams necessarily grouped together is enormous -- in fact infinite, of course -- and, as stressed above, not easy to otherwise intuit in advance.

If it were possible to perform exact calculations, one would of course never need to rely on the techniques described here. The real power of the method becomes apparent however as soon as one needs to approximate -- as one must inevitably do in realistic cases. The mere fact that the exponential form of the wavefunction has real *physical* meaning, now readily lends itself to approximation schemes based on the physics behind it rather than on mathematical convenience or other such spurious reasons. For instance, one may argue that for relatively "low-density" and/or relatively "weakly-interacting" systems, only comparatively rarely do more than n mutually correlated particles lift themselves simultaneously out of the Fermi sea, where we have in mind that n may be as low as 2 or 3. This results in the so-called "natural" or SUB n approximation hierarchy in which all S_m -operators with $m > n$ are set to zero, and the remaining n coupled equations (2.10b) are solved as accurately as possible. This approach has proven immensely successful for atomic and molecular, and nuclear systems.

We point out here that even at the SUB2 level (to go beyond the SUB1 level with $S_1 = 0$, say, and the resulting Hartree-Fock orbitals), an immense

amount of physics is retained. For example, the SUB2 approximation contains as drastic sub-approximations to itself, such other familiar approximations as: (i) the Bethe-Goldstone approximation which sums the so-called particle-particle "ladder diagrams" that describe the scattering of two particles inside the many-body medium; (ii) the analogous Galitskii approximation which also includes all hole-hole and mixed particle-particle/hole-hole ladder terms (and which is further discussed in Section 5); and (iii) the random-phase approximation. The SUB2 approximation also contains terms which incorporate the effects on the intermediate scattering states (in the above cases for example) of the fact that the particles and holes both move in the (self-consistent) potentials due to the rest of the medium. Thus, also (iv) the whole of the usual Brueckner-Bethe-Goldstone theory applied so often to nuclear matter and finite nuclei, for example, is imbedded in SUB2 approximation too. Furthermore, the SUB2 approximation is richer even than the *fully self-consistent* union of all of the above approximations and effects: it also contains classes of (v) particle-hole ladder terms and (vi) extra exchange effects to preserve overall antisymmetry. For further details however we must refer to the literature, and particularly to I. We stress only that SUB2 approximation contains all possible pairing correlations, of the most general type, and the only approximation made is of ignoring their coupling to higher correlations, and hence to composites of more than two particles.

3. Excited-State Coupled Cluster Formalism

The g.s. formalism already described presumably may be employed not only for the g.s. but also for all of those states with the same relevant quantum numbers (or imposed symmetry) as the g.s. that have non-zero inner product with the model state $|\phi\rangle$. We note that Eqs. (4) and (6) automatically provide a normalization $\langle\phi|\psi\rangle = 1$ (and since $\langle\phi|\phi\rangle = 1$, hence $\langle\psi|\psi\rangle \neq 1$). To proceed, we may therefore with no loss of generality restrict ourselves to excited states $|\psi\rangle$ which are orthogonal to both $|\phi\rangle$ and $|\psi\rangle$. Emrich [12] has then shown that an appropriate (linked) choice of excited-state (e.s.) CCF wavefunction is,

$$|\psi\rangle = S^{(\lambda)} e^S |\phi\rangle ; \quad S^{(\lambda)} = \sum_1^N S_n^{(\lambda)} ,$$

$$S_n^{(\lambda)} = \frac{1}{(n!)^2} \sum_{\substack{\rho_1 \dots \rho_n \\ \nu_1 \dots \nu_n}} a_{\rho_1}^+ \dots a_{\rho_n}^+ \langle \rho_1 \dots \rho_n | S_n^{(\lambda)} | \nu_1 \dots \nu_n \rangle_A a_{\nu_1} \dots a_{\nu_n} . \quad (11)$$

Each non-zero vector $S_n^{(\lambda)} |\phi\rangle$ is assumed to have a non-zero inner product with $|\psi\rangle$.

The formal derivation of the e.s. CCF equations is now again easily performed. The e.s. Schrödinger equation,

$$H|\psi\rangle = (E + \omega_\lambda) |\psi\rangle , \quad (12)$$

with excitation energy ω_λ above the g.s. energy E , is first combined with its g.s. counterpart (3), to give

$$[H, S^{(\lambda)}] |\psi\rangle = \omega_\lambda S^{(\lambda)} |\psi\rangle . \quad (13)$$

A similar procedure as in the g.s. case then leads to the linked CCF e.s. equations,

$$\langle \phi_n(\rho, \nu) | e^{-S} [H, S^{(\lambda)}] e^S | \phi \rangle = \omega_\lambda \langle \rho_1 \dots \rho_n | S_n^{(\lambda)} | \nu_1 \dots \nu_n \rangle_A , \quad (14)$$

using the notation of Eq. (9), as the counterparts of the g.s. equations (10b). We note that equations (14) take the form of a coupled set of *linear* eigenvalue equations for the e.s. subsystem amplitudes, with the *same* (excitation energy) eigenvalue ω_λ in each equation, and where the g.s. solution is assumed already known so that the g.s. correlation amplitudes are input to Eqs. (14).

Just as in the g.s. case, the e.s. Eqs. (14) also have to be truncated to be useful in practice. As an obvious extension of the g.s. SUB n scheme, for example, we mention only the SUB(m, n) scheme where the n lowest g.s. equations (10b) and the m lowest e.s. equations (14) are solved in the approximation that the operators $S_{m+k}^{(\lambda)}$ and S_{n+k} are set to zero for all $k \geq 1$.

4. Further Discussion of the CCF

Continuing the discussion of the last Section, an obvious point that arises immediately is the choice of "compatible" (m, n) pairs. For example, one would like to know *a priori* whether for a given n , higher values of m in this SUB(m, n) scheme necessarily lead to better approximations. Such questions are difficult to answer without further information. Very recently, it has however been shown [13] that by imbedding the theory of linear response within the CCF, a set of exact "subsum rules" can be derived. These are essentially cluster decompositions of the more well-known energy-weighted sum rules for the moments of the usual dynamic liquid structure function, and it is shown in Ref. [13] how they can be used as a bridge between the otherwise essentially disparate g.s. and e.s. formalisms presented above. Work is currently in progress to exploit these new tools.

At this point, we recall that the only restrictions (and differences) imposed on the g.s. and e.s. formalisms are (i) $\langle\phi|\psi\rangle \neq 0$, and (ii) $\langle\phi|\psi\rangle = 0$. We have never demanded that $|\psi\rangle$ be approximately given by $|\phi\rangle$, *i.e.* that the matrix elements of the S_n -operators are small, although as already observed in Section 2, the g.s. calculation is likely to converge best if this is true. It is important to note that $|\psi\rangle$ need not in fact be the true ground state of the system. The state $|\psi\rangle$ may be *any* state for which $\langle\phi|\psi\rangle$ happens to be nonzero for the particular model state $|\phi\rangle$ chosen as starting-point. This is a simple but important point for our present purposes, since the calculation of the *true* g.s. may well turn out to be more complicated than for some other exact state $|\psi\rangle$. Similarly, it may also transpire that certain excited states are more readily calculated in the form $S^{(\lambda)} |\psi\rangle$ of Eq. (11) for $|\psi\rangle$ not the true g.s. but some other exact state. In general, of course, it will not be known whether the state $|\psi\rangle$ calculated as in Section 2 with a given $|\phi\rangle$, is indeed the true g.s. or not. In such cases, Emrich [12] has observed that one can use the e.s. formalism of Section 3, and particularly Eq. (14), to seek for states $|\psi^{(\lambda)}\rangle$ with "negative excitation energy" ($\omega_\lambda < 0$). That such states arise in the e.s. rather than the g.s. formalism, is purely an artefact of our initial state $|\phi\rangle$, and we shall henceforth call them "de-excited states".

It is clear from the above description that the many-body states generated by our formalism will depend quite crucially on the choice of zero-order state $|\phi\rangle$,

and indeed this choice will affect whether the given exact state is to be generated by the g.s. or e.s. formalism, as we have just seen. The choice of $|\phi\rangle$ will also be bound up in practice with the realization that the whole scheme is likely to work best when the matrix elements of the S_n -operators are small. In turn, the best choice of $|\phi\rangle$ will depend not only on the system but on which particular phase is under consideration. This point has been particularly stressed and well-illustrated by Zabolitzky [14]. Thus in infinite systems we can define (at least) such four different phases as solid, fluid, superfluid, and clustered. The first three of these are familiar, whereas examples of the clustered phase are the low-density phase of liquid ${}^4\text{He}$ which comprises droplets of several ${}^4\text{He}$ atoms forming a fluid, or the low-density alpha-matter phase of nuclear matter wherein the nucleons bind into (alpha-particle) 4-composites, which form a fluid.

In general, for given density, it is not known beforehand which phase is energetically favoured to be the true g.s., and indeed this is one of the primary questions for a full many-body treatment. Usually one simply makes either an explicit or an implicit assumption. For example most calculations on nuclear matter simply use from the outset that the true g.s. is expected to be homogeneous (translationally-invariant), and hence use plane-waves as the s.p. basis for $|\phi\rangle$. On the other hand, if we were interested to calculate the solid phase, it would make much more sense to start with a zero-order state $|\phi\rangle$ which incorporates the localization at lattice sites of the particles, since this is such a distinguishing and important feature of this phase. In this case one could use localized s.p. states [15] centred on the sites of a particular lattice chosen *a priori*, as being an intuitively obvious starting point. If, on the other hand, one persisted in approximating a solid by starting from the plane-wave $|\phi\rangle$ more appropriate to the fluid, it seems likely that not only would one get much larger S_n amplitudes but also, because the solid is archetypical of a system with long-range order, that if the implied many-body correlations are not present in $|\phi\rangle$ from the outset then also one would need to include S_n -operators with much higher values of n to build up these correlations. In general of course one may calculate the (g.s.) energy starting with both choices of $|\phi\rangle$, but there is no good theoretical reason why either calculation should necessarily exhibit instability against the other phase even if that other phase is of noticeably lower energy. Against this pessimistic view however are the very precise calculations on the one-component Coulomb plasma ("electron gas") [10] which employ the fluid, plane-wave $|\phi\rangle$, and yet even in SUB2 approximation give a g.s. energy at least qualitatively appropriate to the Wigner crystal phase. In this case we imagine that even though the state $|\psi\rangle$ is bound to have the same symmetry, namely translation-invariance, as $|\phi\rangle$ and hence also to be a momentum-eigenstate, then although our calculation cannot break this symmetry it does "next best" and produces an "amorphous solid" (or "liquid crystal") phase.

It is worth pursuing this question of symmetries further. In most cases the zero-state $|\phi\rangle$ will violate some symmetries. For example, any determinant $|\phi\rangle$ built out of s.p. states which are not plane waves, will not be an eigenstate of the linear momentum operator \hat{P} . But on the other hand we know that the representation of Eq. (4) is in principle an exact one and hence eigenstates of both \hat{P} and \hat{H} must be obtainable in this way. In principle this is achieved by also imposing the condition,

$$e^{-S} \hat{P}_e S |\phi\rangle = \hat{P} |\phi\rangle \quad (15)$$

but in practice the series for S in Eq. (4) is curtailed, and Eq. (15) cannot then be imposed exactly. A similar condition to (15) may also be imposed for any other exact symmetry of the phase in question.

On the other hand, this violation of symmetries by model states $|\phi\rangle$ can be put to very good effect. In general, if $|\phi\rangle$ is not an eigenfunction of some symmetry operator \hat{O} that commutes with \hat{H} , it must be a linear superposition of such eigenfunctions, and such wavefunctions often have components which well reproduce the effects of high order correlations. A well-known example of this is the famous BCS wavefunction which includes the effects of Cooper pairing, and gives a very successful zero-order explanation of superfluidity, although it does not conserve particle number. This (symmetry-violating) determinant has in turn been used in the CCF by Emrich [16] as a new model state $|\phi\rangle$ for a more refined theory of superfluidity.

In summary, it is often possible to simulate higher-order correlation effects with a given starting determinant $|\phi\rangle$, by a new choice of determinant $|\phi'\rangle$ (which will often violate certain symmetries of the hamiltonian) which acts as a vacuum for a new set of creation and destruction operators (a_i') and a_i' . In this case the correlations S' in the "exact wavefunction" $|\psi\rangle = \exp(S') |\phi'\rangle$ may now be "smaller", such that a low-order truncation is permissible, whereas in the original basis one needed to go to much higher orders for a good description of *this particular phase*. As we have already observed, we will in general produce in the g.s. CCF, only the g.s. of a given phase corresponding to the symmetries or properties of the particular $|\phi\rangle$ chosen, and the only way to produce the true g.s. is to calculate for all possible phases, and to determine which has minimum energy for given density. But to do this requires a knowledge about all possible phases, and it is therefore of crucial importance to search for other possible phases. There are two distinct ways of doing this. One is to search for new zero-order starting wavefunctions $|\phi\rangle$, perhaps by seeking new solutions of the (generalized) Hartree-Fock equations [17], which may violate certain symmetries. The other, which we now stress, is to look for a given $|\phi\rangle$ and given g.s. CCF solution for "de-excited" states in the e.s. CCF as already mentioned, which are compatible in approximation with the g.s. input. We report very briefly below on some preliminary calculations of this kind.

5. Pairing Correlations and Bound Pairs

We now wish to bring together the discussions of Sections 1 and 4 by focussing particular attention within the CCF on the problem of pairing and composite pairs within a many-fermion system. From previous discussions it seems clear that we should thereby lose nothing by working in the SUB(2,2) approximation in the language of Section 3. Furthermore, since we are primarily interested in new phases, the discussion of Section 1 leads us to focus primary attention on Type I (particle-particle and/or hole-hole) pairing. Thus, starting from the SUB2 approximation for S_2 , we now retain only those terms responsible for generating the complete sum of ladder diagrams for two-particle/two-hole scattering in the many-body medium, *i.e.* the particle-particle (pp), hole-hole (hh) and mixed pp-hh ladders. This leads to what we call the complete ladder (CLAD) equation, completely equivalent to the Galitskii approximation of the two-body Green function in the time-dependent perturbation theory approach.

The CLAD approximation in the g.s. CCF may be

formally arrived at by keeping only the first two terms on the right-hand side of the otherwise *exact* Eq. (2.10) of I for S_2 , and otherwise keeping only the (bare) kinetic energies for the hole-energy terms given by Eq. (2.11) of I in the left-hand side of Eq. (2.10) of I. In our compact notation, the basic CLAD equation may then be written as

$$e_0 \langle \rho_1 \rho_2 | S_2 | v_1 v_2 \rangle_A = - \langle \rho_1 \rho_2 | V(1+S_2) | v_1 v_2 \rangle_A - \frac{1}{2} \sum_{v, v'} \langle \rho_1 \rho_2 | S_2 | v v' \rangle_A \langle v v' | V(1+S_2) | v_1 v_2 \rangle_A, \quad (16)$$

$$e_0 \equiv \epsilon_{\rho_1} + \epsilon_{\rho_2} - \epsilon_{v_1} - \epsilon_{v_2}. \quad (17)$$

In order to work from the fluid-phase as starting-point, we also choose $|\phi\rangle$ to be made of plane-wave s.p. orbitals in the usual way. With an obvious momentum-labelling of the s.p. states, Eq. (16) may be represented diagrammatically by Fig. 2, where the terms (a) - (e) which arise from the right-hand side of

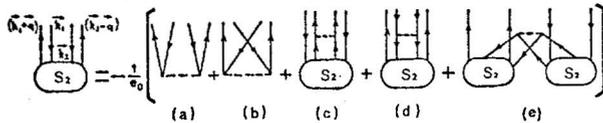


Figure 2: Diagrammatic representation of the g.s. CLAD equation for S_2 . The dashed line represents the bare potential V , and e_0 is given by Eq. (17).

Eq. (16) correspond respectively to diagrams (a), (d), (m), (n) and (o) of the full SUB2 equation of Fig. 1 of I. We note again only that the diagrams are "time-ordered" in the sense of Goldstone perturbation theory, and that s.p. lines with arrows pointing upwards (downwards) are to be strictly associated with particle (hole) states respectively. It is clear by straightforward iteration that in the form expressed by Fig. 2, the diagrams (c) and (d) taken individually generate respectively the complete sets of ladder diagrams for pp and hh scattering in the many-body medium. Similarly the quadratic term of diagram (e) generates the mixed pp-hh ladders. The analogous equation for the e.s. correlation operator $S_1(q)$, which now carries as excitation index the (exactly conserved quantum number) momentum q , is very similarly written down from Eq. (14) in the CLAD-truncated SUB(2,2) scheme (with $S_1 \neq 0$ by momentum conservation, and $S_1(q) = 0$ by fiat for the CLAD sub-approximation), or, most simply, by exploiting the "[g-e] symmetrization" of Emrich [12].

In the momentum representation, Eq. (16) is a non-linear integral equation. It has been found possible to solve both it and its e.s. analogue exactly in SUB(2,2) and CLAD approximation, for the simple model where the two-body potential operator takes the form $V = \lambda |g\rangle\langle g|$ of a one-term, S-wave, separable potential. The solution in many ways is rather similar to the analogous RPA solution reported in I for a local potential, although the details are far too complex to discuss here and will be reported elsewhere [18]. We emphasise only that the various types of composite or bound (Type I) pairs within the many-body medium now manifest themselves very naturally within the g.s. CCF as "virtual (de-)excitations" in the exact g.s. solution for S_2 . These (de-)excited states are then also seen explicitly in the exact e.s. solution, where their

wavefunctions within these approximations can be exactly solved for. In the g.s. CCF the (de-)excited Type I pair states show up "virtually" as poles in the suitably analytically-continued matrix elements of S_2 , in complete analogy to the plasmon (Type II) pole observed in the g.s. CCF in random-phase approximation, and as discussed in I in great detail.

Without going into the analytic details of the solutions, we report only the qualitative nature of the results obtained. We find that the CCF does indeed provide, even in this simple CLAD approximation, an efficient and unified framework in which to describe all aspects of Type I pairing. In particular we find in this single calculation: (i) a possible free bound pair (for sufficiently attractive potentials; e.g. the deuteron in the nuclear matter case) and its gradual approach to "dissolution" as the density is increased; (ii) the possible appearance of a second bound pair of predominantly hole-like quasiparticles above a lower critical density (for given total pair momentum); (iii) the unstable but bound resonant pairs that can exist for densities above a comparable upper critical density at which the two previous real bound pairs have "dissolved"; and (iv) Cooper pairs. Even though each of these composite pairs leads to a new "condensed-pair phase" of lower energy for appropriate densities, the so-called g.s. CCF built here on the plane-wave $|\phi\rangle$ leads only to the fluid-like state of uncondensed particles. The various composite pairs materialize in the e.s. CCF as (negative energy) (de-)excited states. Thus, types (i) and (ii) above lead to the clustered phase of, for example, deuteron matter as a low-density phase of nuclear matter; type (iii) leads to the (unstable) continuation of the clustered deuteron-matter phase into the density range where the fluid phase is not yet energetically favoured (at this level of approximation); and type (iv) leads to the superfluid phase.

6. Conclusions and Future Developments

From the above results, it is clear that a judicious and compatible choice of g.s. and e.s. CCF approximations can indeed lead to the *possibility* of new phases, starting from a *given* (in this case, fluid-like) model state $|\phi\rangle$. The e.s. formalism shows how to obtain *single* composite pair states of lower energy than the g.s. obtained in the same approximation. In order to exploit fully the power of the method one should as a next step start with a new model state $|\phi'\rangle$ which exploits these composite pairs so obtained. Thus, for example, for the type (iv) Cooper pairs, one could for $|\phi'\rangle$ use the usual BCS state, as discussed in Ref. [16]. Similarly, for the deuteron clustered phase of nuclear matter, one should now build up a new $|\phi'\rangle$ from the composite pairs of types (ii) and (iii) already found. This step has not yet been done but we hope to do so in the future.

Also of interest is to extend the CLAD calculations here to a full SUB(2,2) approximation, and thereby to examine the interference on the Type I composite pairs reported here of the so-far neglected remaining terms in the full SUB(2,2) equations, some of which are themselves largely responsible for the Type II pairs or collective excitations.

Finally, we are also interested in extending the present approach to at least a qualitative enquiry into the analogous various possibilities of bound three- and four-body clusters, and the consequent possible condensed phases associated with them.

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