Towards a universal coupled cluster methodology for the various phases of condensed matter systems

Document Version
Accepted author manuscript

Link to publication record in Manchester Research Explorer

Citation for published version (APA):
Bishop, RF. (1987). Towards a universal coupled cluster methodology for the various phases of condensed matter systems. In P. J. Siemens, & R. A. Smith (Eds.), Recent Progress in Many-Body Theories (pp. 1-12). Texas A&M University.

Published in:
Recent Progress in Many-Body Theories

Citing this paper
Please note that where the full-text provided on Manchester Research Explorer is the Author Accepted Manuscript or Proof version this may differ from the final Published version. If citing, it is advised that you check and use the publisher's definitive version.

General rights
Copyright and moral rights for the publications made accessible in the Research Explorer are retained by the authors and/or other copyright owners and it is a condition of accessing publications that users recognise and abide by the legal requirements associated with these rights.

Takedown policy
If you believe that this document breaches copyright please refer to the University of Manchester's Takedown Procedures [http://man.ac.uk/04Y6Bo] or contact uml.scholarlycommunications@manchester.ac.uk providing relevant details, so we can investigate your claim.
published in:

"Recent Progress in Many-Body Theories,"
(eds. P.J. Siemens and R.A. Smith),
Texas A & M University,
College Station, 1987, 1–12
TOWARDS A UNIVERSAL COUPLED CLUSTER METHODOLOGY FOR
THE VARIOUS PHASES OF CONDENSED MATTER SYSTEMS

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

1. INTRODUCTION

In this paper we review the coupled cluster formulation of quantum many-body theory. Apart from a brief and heuristic, but essentially complete, discussion of the by now rather standard treatments of both ground and excited states within the coupled cluster method (CCM), our main aim is to give a rather careful critique of the various choices that have to be made in order to implement the method. These divide essentially into two classes. On the one hand we have the inputs to the method, which amount largely to a choice of starting (or zero-order or model or uncorrelated) wavefunctions; while on the other hand we have the choice of decomposition of the equations into a natural hierarchy, and which amounts in practice to a particular approximation or truncation scheme. We shall show explicitly that while these two choices are in principle independent of each other, in practice they are intimately connected. It is clear that in practice particular choices must depend not only on the individual physical system but also on which of its possible phases is under study.

Of particular interest to us here is to what extent the CCM and its various starting and truncation scheme choices can be turned into a universal machine. That is, we are interested in how far the coupled cluster methodology can be made complete and self-consistent, to the extent both of iterating the CCM (with given initial choices to implement it) to generate better or more appropriate (for a given phase of a given system) wavefunctions and truncation schemes, and of generating all possible phases of a given system without prior knowledge of them. We illustrate our discussion by considering the problem of generalized pairing within a many-fermion system as an example of the more general phenomenon of the possible formation of bound composite clusters in condensed matter systems, and the associated macroscopic phases which ensue from them.

2. COUPLED CLUSTER METHODOLOGY FOR THE 'GROUND STATE'

We consider a system of N identical fermions whose mechanics is governed by the nonrelativistic Schrödinger equation with a hamiltonian $H$ that comprises a sum of one-body (kinetic energy) terms, two-body interaction potential terms, and in general also three- (and more) body potential terms.
2.1 Cluster decomposition of the wavefunction.

The starting-point for the ground-state (g.s.) CCM is to express the exact g.s. N-body wavefunction \( |\Psi\rangle \), in terms of some starting (or model or reference) wavefunction \( |\phi\rangle \), in the form,

\[
|\Psi\rangle = e^S |\phi\rangle ; \quad S = \sum_{n=1}^{N} S_n,
\]

where the correlation operator \( S \) in general contains \( n \)-body contributions \( S_n \) for all \( n = 1, \ldots, N \) as indicated. The wavefunction \( |\phi\rangle \) may in general itself be a rather complicated (highly correlated) object. It is by no means necessary that it is an eigenfunction of some appropriate zero-order hamiltonian \( H_0 \). However, purely for simplicity of future discussion, we restrict ourselves henceforth to the choice of an (uncorrelated) single Slater determinant form for \( |\phi\rangle \). Thus, defining the operators \( a_\alpha^+ \) to be a set of fermion creation operators for the (arbitrary) complete and orthonormal single-particle (s.p.) basis states \( |\alpha\rangle = a_\alpha^+ |0\rangle \), with \( |0\rangle \) the vacuum state, we choose

\[
|\phi\rangle = a_1^+ \ldots a_N^+ |0\rangle. \quad (2)
\]

Henceforth we adopt the standard notation that s.p. labels \( \nu_1 \) indicate states included in \( |\phi\rangle \), and which when vacated correspond to "hole states" in the usual terminology; whereas the remaining s.p. states not included in \( |\phi\rangle \) are called "particle states", and given the labels \( \rho_1 \). (We note parenthetically that it is easy to envisage physical systems where a linear superposition of several Slater determinants might appear to be a "better" starting wavefunction, or indeed where no such superposition of Slater determinants seems \textit{a priori} intuitively reasonable. One of our main aims is a critical discussion of such intuitive ideas, when more rigorously formulated).

In second-quantized form, the operators \( S_n \) may be expressed as,

\[
S_n = \frac{1}{n!} \sum_{\nu_1 \ldots \nu_n} \langle \rho_1 \ldots \rho_n | S_n | \nu_1 \ldots \nu_n \rangle a_\nu_1^+ \ldots a_\nu_n^+ a_{\rho_1} \ldots a_{\rho_n}, \quad (3)
\]

where we have used the notation \( |\nu_1 \ldots \nu_n\rangle = |\nu_1\rangle \ldots |\nu_n\rangle \) is the ordered (non-antisymmetrized) direct product state. Equation (3) expresses the fact that the \( S_n \) are n-particle/n-hole correlation operators, which as far as Eq. (1) is concerned have non-vanishing matrix elements only for creating \( n \) particle and \( n \) hole states on top of \( |\phi\rangle \). In other words, the operators \( S_n \) have vanishing matrix elements, \( \langle \ldots \nu | S_n | \ldots \rangle = 0 \), for re-filling any of the \( n \) holes first created in \( |\phi\rangle \).

The real content of the exponential form of the wavefunction \( |\Psi\rangle \) given in Eq. (1) is that the matrix elements of the operators \( S_n \) in Eq. (3) are connected. Thus, for example, \( S_6 \) contains no pieces which describe the behaviour of two independent (or disconnected) 3-particle/3-hole excitations from \( |\phi\rangle \). A rather complete heuristic and pedagogical interpretation (and derivation) of the exponential form of the wavefunction in Eq. (1) has been given elsewhere recently, and will not be repeated here.
The g.s. coupled cluster equations may now most readily be expressed by first writing the g.s. Schrödinger equation, with energy eigenvalue $E$, in the form

$$e^{-SHe^S}|\phi\rangle = E|\phi\rangle.$$  \hspace{1cm} (4)

The operator product in the left-hand side of Eq. (4) has the well-known expansion,

$$e^{-SHe} = H + [H,S] + \ldots + \frac{1}{n!}[[[H,S],S],\ldots,S] + \ldots,$$  \hspace{1cm} (5)

which involves the nested commutators of $H$ once with $S$ an arbitrary number of times. For a given $N$-fermion hamiltonian containing no higher than, say, $k$-body interaction potentials, one readily sees that the otherwise infinite expansion (5) actually terminates at the term involving at most $2k$ $S$-operators. When each $S$-operator is in turn expanded into its $n$-body pieces $S_n$ from Eq. (1), the mutual commutativity of these pieces (as immediately implied by Eq. (3)) then guarantees that all remaining terms are "connected" or "linked" to the Hamiltonian. This has the effect of by-passing the usual "size-consistency problem." That is, all (macroscopic) terms which scale like $N$ or some finite positive power of $N$, are eliminated from the otherwise microscopic equations, with the exception only of those terms that contribute to the energy $E$ itself to yield equality with the right-hand side of Eq. (4).

Finally, Eq. (4) is decomposed by projecting it onto either the model state $|\phi\rangle$ or onto those $n$-particle/n-hole states,

$$|\phi_n^{p_1,\ldots,p_n,v_1,\ldots,v_n}\rangle = a_{p_1}^+ \ldots a_{p_n}^+ a_{v_1} \ldots a_{v_n} |\phi\rangle,$$  \hspace{1cm} (6)

built on it. The states $|\phi\rangle$ and $|\phi_n\rangle$, $n = 1,\ldots,N$, span the entire $N$-body Hilbert space when the labels $p_i$ and $v_i$ span the complete s.p. basis, as assumed. Thus, the g.s. coupled cluster equations,

$$\langle\phi|e^{-SHe^S}|\phi\rangle = E;$$

$$\langle\phi_n^{p_1,\ldots,p_n,v_1,\ldots,v_n}|e^{-SHe^S}|\phi\rangle = 0; \hspace{0.5cm} n = 1, \ldots, N,$$  \hspace{1cm} (7)

are fully equivalent to the original $N$-body Schrödinger equation and are just a (truly microscopic) cluster decomposition of it. Further evaluation of Eqs. (7) is straightforward although algebraically tedious. Explicit derivations for the cases $n = 1$ and 2 have been given,\(^2\) and for further details and applications the reader is directed to recent review articles.\(^3\)\(^-\)\(^6\)

We remark finally that the only places where one needs to inject physical intuition into practical applications of the formalism are choices for (i) the Slater determinant $|\phi\rangle$, and (ii) the approximation scheme to truncate the coupled set of Eqs. (7). We address ourselves in turn to these related points.

2.2 Choice of starting wavefunction $|\phi\rangle$

From our previous discussion it is clear that if the formalism were carried out exactly (to all orders $n$ for example), the results would be independent of $|\phi\rangle$.

Conversely when we make approximations, as we always must in practice, the dependence
of any results on $|\phi\rangle$ should be weak. This in turn can be used as an internal consistency check on the quality of the results.

Intuitively we may feel that the "closer" is $|\phi\rangle$ to the exact $|\psi\rangle$, and correspondingly the "smaller" is the correlation operator $S$, the better is that choice for $|\phi\rangle$ likely to be at a given level of approximation. Alternatively, we may intuit that if $|\phi\rangle$ shares the same underlying symmetries or breaks the same symmetries as the exact $|\psi\rangle$, the better is it likely to be. It is clear that both of these statements depend critically not only on the system under consideration but also on which particular phase is stable for given values of the adjustable parameters. As we have already indicated, herein lies the rub, since one of our principal goals is not only to derive the various regions of stability but also the various phases themselves.

Before returning to this crucial point however we pursue each of these two intuitive lines of thought further.

The first idea has been formulated and quantified by Kümme17 as the maximum overlap condition,

$$ J = \frac{|\langle \phi' | \psi \rangle|^2}{\langle \phi' | \phi' \rangle < \langle \psi | \psi \rangle >} = \text{maximum}, $$

(8)

which is to be implemented by varying $|\phi'\rangle$ over all Slater determinants for fixed $|\psi\rangle$. If $|\phi\rangle$ is the maximizing wavefunction, the well-known theorem of Thouless ensures that any other $|\phi'\rangle$ in the vicinity of (and hence not orthogonal to) $|\phi\rangle$ has the representation

$$ |\phi'\rangle = \exp(T_1) |\phi\rangle, $$

(9)

where $T_1$ is a 1-particle/1-hole excitation operator of similar form to $S_1$ of Eq.(3). (The Thouless theorem similarly shows that the $S_1$ operator in Eq. (1) plays the special role of permitting us to shift from one arbitrary s.p. basis to another). The functional $J$ of Eq. (8) is then maximized by expanding it in powers of the matrix elements $<\phi | T_1 | \psi>$ out to second order. The necessary (extremal) condition is then that the first order variation should vanish. One can readily show that this leads to the result,

$$ S_1 = 0. $$

(10)

Inserting $S_1 = 0$ into the 1-body g.s. CCM-equation -- namely Eq. (7) with $n = 1$ -- then gives an equation for the optimal s.p. basis under criterion (8). If furthermore we restrict ourselves to the approximation where higher correlations are zero ($S_n = 0$, $n \geq 2$) this reduces precisely to the Hartree-Fock (HF) equation. Otherwise the equation is exact and defines a generalization of the HF orbitals.

We note that the condition (10) is only a necessary condition. There is also a sufficiency condition which comes from the second order variation with respect to the elements $<\phi' | T_1 | \psi>$, and which ensures that the extremum is indeed a maximum rather than a minimum. Kümme17 shows explicitly how this extra condition depends on the size of the correlations. Specifically if one considers the eigenvalues $\sigma_1$ and eigenvectors $X_{1}^{(1)}$ of the matrix $S_2$ in the space of 1-particle/1-hole states, via
the secular equation,

\[ \sum_{\rho',\nu'} \langle \rho' | S_2 | \nu' \rangle A \langle \rho' | X_i^{(i)} | \nu' \rangle = \sigma_i \langle \rho | X_i^{(i)} | \nu \rangle, \]  

(11)

one can show that the sufficient condition for \( J \) to be a maximum is,

\[ \sigma_i^2 < 1, \text{ all } i. \]  

(12)

This relation quantifies what we previously intuited, namely that the correlations imposed by the operator \( S \) in Eq. (1) should be small for a reasonable choice of \( |\phi\rangle \).

It is particularly noteworthy that only the pair correlation operator \( S_2 \) plays a role here. One could imagine exploiting condition (12) to search for critical points as a function of the relevant external parameters \( \{\lambda\} \) built into \( |\phi\rangle \) or \( H \). Thus we imagine that \( |\sigma_i^{(i)}(\lambda)\rangle + 1 \) as \( \{\lambda\} \rightarrow \{\lambda_c\} \) for some \( i \), and that at this critical point in the parameter space \( \{\lambda\} \) we have a shape or phase transition to a different configuration \( |\phi\rangle \). To date this approach has scarcely been utilised in practice, but we believe that potentially its use could be of great importance in our search for a "universality programme" for the CCM.

In practice a shape or phase transition as envisaged above is likely to be accompanied by some change of symmetry of \( |\psi\rangle \). This is intimately connected with our second intuitive point above -- that a good \( |\phi\rangle \) should share the same underlying symmetries as \( |\psi\rangle \). These will in turn depend on the phase under consideration. Thus in infinite systems we can define (at least) the four different types of phase: solid, fluid, superfluid, and clustered. Generally we have no a priori knowledge of which phase is the true g.s. for given system parameters \( \{\lambda\} \), and some explicit or implicit assumption is usually made. For example, most calculations on nuclear matter impose from the outset that the true g.s. is expected to be homogeneous (fluid), and hence use plane waves as the s.p. basis. On the other hand, such a Slater determinant \( |\phi\rangle \) of plane waves makes much less obvious sense as a starting wavefunction for the solid phase. For this case one imagines that the correlations would now be much larger and, worse, since the solid phase has long-range order that correlations \( S_n \) with very large values of \( n \) might be needed.

In practice one could imagine putting the g.s. CCM into effect for a range of starting wavefunctions \( |\phi\rangle \), each of which is tailored to a particular phase, guessed beforehand as being possible, and calculating the g.s. energy for each. We might then hope that at some \( \{\lambda_c\} \) the (approximate) calculation on phase A (built on some \( |\phi_A\rangle \) should exhibit instability against another approximate calculation for phase B. However there is simply no compelling theoretical reason why this must occur, even when the separate calculation gives noticeably lower energy for phase B. (Against this pessimistic view however is some pragmatic evidence obtained for the electron gas, within the CCM based on a \( |\phi\rangle \) built of plane waves, where at low densities definite signs of a phase transition to crystallization are observed.)

In most cases, the states \( |\phi\rangle \) will violate some symmetries of the exact \( |\psi\rangle \) which can certainly be restored with an exact \( S \) of the form of Eq. (1), but not
necessarily with a truncated one as might be used at a given level of approximation.

Paradoxically, this violation of symmetries can often be turned to our advantage. In general if $|\psi\rangle$ is not an eigenfunction of some symmetry operator $\Theta$ that commutes with $H$, it must be a linear superposition of such eigenfunctions, and such wavefunctions often have components which reproduce rather well the effects of higher order correlations, that one might otherwise miss altogether in a given truncation of the CCM equations with a single eigenfunction form for $|\psi\rangle$. A famous example is the BCS wavefunction which gives a successful zero-order account of superconductivity but which violates particle number conservation.

Ultimately however we do require a knowledge about all possible phases of a given system, and it is of crucial importance to search systematically for these. We return to this point after a discussion of the excited-state (e.s.) CCM.

2.3 Approximation schemes

Once having settled on a choice of starting wavefunction $|\psi\rangle$, we still need to approximate the otherwise exact hierarchy of CCM equations (7). It is clear that in principle the approximation scheme should be tailored both to the particular system and to the choice $|\psi\rangle$. The fact that the exponential form of the wavefunction in Eq. (1) has real physical significance is now important in that approximation schemes based on it may be expected to have physical relevance rather than simply mathematical ease. For instance, one can argue that for relatively low-density and/or relatively weakly-interacting systems only rarely do more than $n$ particles come together to lift themselves out of their s.p. orbitals assigned to them in $|\psi\rangle$, where we have in mind that $n$ may be as low as 2 or 3. This results in the so-called "natural" or $SU_B \eta n$ approximation hierarchy in which all $S_m$ operators with $m > n$ are set to zero, and the remaining $n$ coupled equations (7) are solved as exactly as possible. This approach has been described fully elsewhere, and has met with great success in applications to the electron gas and in quantum chemistry, for example.

Alternatively, the so-called Bochum (or $\chi^n$) truncation scheme has been successfully applied where the interparticle forces contain a very strong repulsive core as in nuclear physics. The guiding principle here is that the particles must stay largely outside their core region of mutual strong repulsion and yet still have only relatively few particles clustering together on average at a time. For further details we refer the reader to the literature.

It is however still true that some guesswork is needed at this stage to tailor an approximation scheme to a particular $H$ and $|\psi\rangle$. The present state of the art is that there is now a considerable body of experience on which to draw for a wide variety of systems. It is however likely that new (and perhaps more sophisticated) approximations will be needed to treat more complex or more subtle problems. There will always in this context be a competition between the complexity of $|\psi\rangle$ on the one hand and the sophistication of the approximation scheme on the other. Thus, any shortcomings in the one can be compensated by the other. We return to this point later.
We note for the moment only that for any application, there are always two internal consistency checks, namely: (i) that the dependence of the results on the parameters of $|\phi\rangle$ for a given approximation should be weak; and (ii) that, for a given $|\phi\rangle$, the results should (rapidly) converge as one moves to higher levels of approximation within a given truncation scheme.

3. COUPLED CLUSTER METHODOLOGY FOR 'EXCITED STATES'

Although the CCM presented in Section 2 has been referred to as the g.s. formalism, there was never any restriction which forced $|\psi\rangle$ to be the exact ground state of $H$ for given values $(\lambda)$. The only restriction placed on $|\psi\rangle$ by the formalism is that $\langle\phi|\psi\rangle = 0$ -- in fact Eqs. (1)-(3) show that $|\psi\rangle$ is normalized in the formalism by $\langle\phi|\psi\rangle = 1$. Presumably therefore the g.s. formalism should generate all eigenstates of $H$ that have non-zero overlap with the particular model state $|\phi\rangle$. Whether this class of states actually contains the true g.s. for given $(\lambda)$ depends both on our choice of $|\phi\rangle$ and on the nature (phase) of the exact g.s. for such $(\lambda)$. For ease of discussion however, we continue to call the formalism of Section 2.1 the g.s. CCM.

By contrast, all remaining eigenstates of $H$ -- which we now refer to as "excited states" (e.s.) in keeping with the above terminology -- have exact wavefunctions $|\psi_{\lambda}\rangle$ such that $\langle\phi|\psi_{\lambda}\rangle = 0$. For such states, Emrich\(^9\) has shown that an appropriate (linked) choice of e.s. wavefunction within the CCM is,

$$|\psi_{\lambda}\rangle = S(\lambda)e^S|\phi\rangle; \quad S(\lambda) = \sum_{n=1}^{N} S_n(\lambda)$$

$$S_n(\lambda) = \frac{1}{n!} \sum_{\rho_1 \ldots \rho_n} \langle \rho_1 \ldots \rho_n | S_n(\lambda) | \nu_1 \ldots \nu_n \rangle a_1^\dagger \ldots a_1^\dagger a_n \ldots a_n,$$  \hspace{1cm} (13)

where each non-zero vector $S_n(\lambda)|\phi\rangle$ is assumed to have a non-vanishing overlap with the exact $|\psi_{\lambda}\rangle$.

In order to derive the e.s. counterparts of Eqs. (7), it is convenient first to combine the e.s. Schrödinger equation,

$$H|\psi_{\lambda}\rangle = (E + \omega_{\lambda})|\psi_{\lambda}\rangle,$$  \hspace{1cm} (14)

where $\omega_{\lambda}$ is the "excitation energy", with its g.s. counterpart (4), to give

$$e^{-S[H,S(\lambda)]} e^S|\phi\rangle = \omega_{\lambda} S(\lambda)|\phi\rangle,$$  \hspace{1cm} (15)

in which form the g.s. energy $E$ does not appear. Finally by projection onto the $n$-particle/$n$-hole states of Eq. (6), the e.s. counterparts of the g.s. Eqs. (7) are obtained as,

$$\langle \rho_1 \ldots \nu_1 | e^{-S[H,S(\lambda)]} e^S | \phi \rangle = \omega_{\lambda} \langle \rho_1 \ldots \nu_1 | S(\lambda) | \phi \rangle.$$  \hspace{1cm} (16)

The basic structure of the e.s. Eqs. (16) is that they are a coupled set of linear eigenvalue equations for the matrix elements of the operators $S_n(\lambda)$, in which the matrix elements of the g.s. operators $S_n$ are input, having solved Eqs. (7). In
practice Eqs. (16) have to be truncated, just like Eqs. (7), and the problem of compatible approximation schemes between the g.s. and e.s. formalisms arises, and has been discussed elsewhere.\textsuperscript{10}

The question that we now address is whether we can use the e.s. equations to assist with the search for (instabilities associated with) shape/phase transitions. What we have in mind is that if we approach a transition, a model state $|\Psi\rangle$ appropriate to phase A ($\langle\phi|\Psi_A\rangle = 0$) with true g.s. $|\Psi_A\rangle$ may become so bad as to have zero overlap with the true g.s. $|\Psi_B\rangle$ for phase B. In this case, one intuits that $|\Psi_B\rangle$ should appear (with the given $|\Psi\rangle$) as a "de-excited state" in the e.s. CCM, i.e. with negative excitation energy, $\omega \ll 0$. We examine this possibility below for the concrete example of pairing.

4. CORRELATED PAIRS AS DE-EXCITED STATES

There are essentially two different types of (bound) composite bosons that can occur in a system of many identical fermions.\textsuperscript{11} Type I comprise an even number of particles or an even number of their corresponding holes; while Type II comprise bound complexes of particle-hole pairs. Examples of Type I are $^4$He atoms and Cooper pairs; and of Type II are phonons, excitons and the giant resonances in nuclei. The Bose condensation of Type I complexes such as Cooper pairs is accompanied by off-diagonal long-range order in coordinate space and the appearance of a superfluid-like phase. The Bose condensation of Type II complexes, by contrast, leads to diagonal long-range order in coordinate space. Examples of Type II condensation are the excitons in photoexcited semiconductors which lead to the excitonic phase, and the phonons in a crystal which can condense into a single mode and give rise to a distortive phase transition of the crystal, with the appearance of a superlattice.

The appearance of $n$-composites within the CCM can be studied via the correlation operators $S_n$ and $S_2(x)$. As a first example we discuss here a study of the important $n = 2$ case which will incorporate generalized pairing within the many-fermion system. We have chosen to work with the "natural" truncation scheme outlined in Section 3, and hence here in the so-called SUB(2,2) approximation where we solve Eqs. (7) and (16) for $S_2$ and $S_2(x)$ in the approximation that $S_n = 0 = S_2(x)$ for $n > 2$. Furthermore, for infinite, homogeneous systems (as assumed here) $S_1 = 0$ by momentum conservation; and $S_2(x)$ is set to zero also. In this case, we work with plane waves as our s.p. basis and the excitation index $\omega \ll 0$ is now the (exactly conserved) momentum $q$.\textsuperscript{12}

The remaining SUB(2,2) equations still contain an enormous amount of physics, as described for the g.s. for example in Ref. [2]. In particular they contain terms responsible for both Type I pairing (e.g., all of lowest-order Brueckner-Bethe-Goldstone theory is included) and Type II pairing (e.g., the random-phase approximation is included). Since we are primarily interested here in illustrating the power of the CCM in generating new phases itself from a given starting wavefunction $|\phi\rangle$, it seems sensible as a first step to restrict further attention to, say, Type I pairing.
only. In that case we focus attention as a first step on the sub-approximation of retaining only those terms in the SUB2 equation for $S_2$ which generate the complete set of ladder diagrams for two-particle/two-hole scattering in the many-body medium -- namely, the particle-particle (pp), hole-hole (hh), and mixed pp-hh ladders. This leads to the so-called complete ladder (CLAD) equation, which is itself equivalent to the well-known Galitskii approximation for the two-body Green function in the time-dependent perturbation theory approach. The analogous equation for the e.s. correlation operator $S_2^{(q)}$ is rather easily written down by exploiting the symmetry between the left-hand sides of the g.s. and e.s. Eqs. (7) and (16) respectively, which becomes apparent upon making the expansion in Eq. (5). Further details are given elsewhere.\footnote{1,2}

Using plane waves as the s.p. basis, the SUB(2,2) equations still amount to a very difficult non-linear integral equation for the g.s. $S_2$, and a rather tricky linear eigenvalue problem for the e.s. $S_2^{(q)}$. As a first illustrative example we have used a one-term, S-wave, separable two-body interaction potential, $V = \lambda |g><g|$. In this case, we have shown\footnote{12} how exact analytic results may be obtained. In many ways the solution is comparable for this non-local potential to the analogous solution in random-phase approximation (RPA)\footnote{2} for a local potential. The detailed solution is too long and complex to discuss here but will be fully reported elsewhere.\footnote{12} We report here only on such qualitative results as are important for illustrating the present discussion of the CCM. We find that just as in the case of the electron gas in RPA,\footnote{2} where the g.s. CCM naturally evolves a dielectric function whose zeros play a very special role in the solution, so here a comparable function arises in the g.s. CCM, whose zeros critically determine the exact analytic form of the solution. It is in this way that the various types of composite or bound (Type I) pairs manifest themselves very naturally within the g.s. CCM as zeros or "virtual (de-)excitations" in a two-body g.s. correlation operator. These same states are then seen also in the e.s. CCM solution, where they are explicitly solved for as real "de-excited states" of negative eigen-energy $\omega_q$.

We find, as we had hoped, that the CCM does indeed provide, even in this relatively simple CLAD approximation, a rather efficient and unified framework from which to derive all aspects of Type I pairing. We find that the so-called "ground-state" which emerges from our g.s. CCM calculation, is just a fluid-like state of uncondensed particles. By contrast, the energy may be lower in the e.s. CCM, which in this case represents a (negative energy) de-excited state by comparison with the g.s., corresponding to the formation of a single (Type I) pair.

As an illustration of the results obtained, we consider the (physically most interesting) case of an attractive ($\lambda<0$) potential, strong enough to support a 2-body bound state in vacuo (e.g., the deuteron in the case of nuclear matter). In our single CCM calculation based on a starting wavefunction $|\Phi>$ built of plane-waves, we then find: (i) the gradual dissolution of the "deuteron-like" bound pair as the density of the system increases; (ii) the possible appearance of a second type of bound pair...
of predominantly hole-like quasiparticles, above a lower critical density (for given total pair momentum); (iii) unstable but bound resonant pairs that can exist above a comparable upper critical density at which the two previous real bound pairs have "dissolved"; and (iv) Cooper pairs. It is clear that each of these states can then lead to a new condensed-pair phase in the appropriate-density-range for which they exist. Types (i) and (ii) thus lead to a clustered phase -- e.g., in this approximation, the low-density deuteron-matter phase of nuclear matter; whereas Type (iii) lead to the (unstable) continuation of this phase into the density regime where the fluid phase is still not energetically favoured however at this level of approximation. Finally, Type (iv) pairs clearly lead to a superfluid phase.

Having found such single bound pair states, the next step is clearly (i) to use the pair wavefunctions obtained, from solving for $S_2(q)$, to build a new starting wavefunction $|\psi\rangle$ to model each new phase -- i.e., to have non-zero overlap with the exact $|\psi\rangle$, $\langle\psi|\psi\rangle \neq 0$; and (ii) to perform the g.s. CCM again with each new $|\psi\rangle$. Finally, it is clearly also of interest to extend these CLAD calculations to a full SUB(2,2) approximation, and hence to examine the interplay between the Type I composite pairs discussed here, and the so-far neglected Type II pairs which represent the simplest collective excitations. Furthermore, one can imagine extending these calculations to higher orders, to provide at least a qualitative description of the various possible composite clusters of three and four particles, and their associated macroscopic phases.

5. POSSIBLE INGREDIENTS OF A UNIVERSAL CCM

From our previous discussion of the CCM we stress again the following features:

(i) the many-body states generated depend crucially on the choice of model state $|\phi\rangle$.
(ii) The choice of $|\phi\rangle$ in particular determines whether a given exact state is generated by the g.s. or e.s. CCM. (iii) The "best" choice of $|\phi\rangle$ will depend on which phase of the system is being considered. (iv) For a given set of system parameters $\{\lambda\}$ we do not in advance know which phase is energetically favoured. Usually an implicit assumption is made in constructing $|\phi\rangle$ -- e.g., using plane waves for a fluid phase or a BCS wavefunction for a superfluid phase. (v) We would like the calculation on a given phase (or given symmetry imposed on $|\phi\rangle$) to exhibit instability or some other internal signal of an impending phase transition. (vi) The violation of certain symmetries by $|\phi\rangle$ can often be used to mock up higher order correlations, such that one may be able to work to a lower order of approximation with a "good" symmetry-violating $|\phi\rangle$ than for a symmetry-conserving $|\phi\rangle$.

We will in general produce by the g.s. CCM, only the g.s. of a given phase corresponding to the symmetries or other properties of the particular starting wavefunction $|\phi\rangle$ that we are employing. 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 system parameters $\{\lambda\}$. But to do this requires a knowledge of all possible phases,
and hence a truly universal formalism would itself be capable of generating these.

Our present belief is that two distinct but related routes within the CCM to this goal are:

- **1.** To search for new starting wavefunctions $|\phi\rangle$, e.g., by:
  - (a) exploiting the maximum overlap stability criterion previously discussed;
  - (b) seeking new ("abnormal") solutions of the (generalized) HF equations (discussed previously in connection with the previous point), which perhaps violate certain symmetries. Some work has been done in this direction, but we believe that it is still relatively unexplored territory; and
  - (c) building into $|\phi\rangle$ parameters which when assigned non-zero values break certain symmetries, and with such parameters able to be self-consistently determined within the formalism by putting into effect some appropriate criterion.

- **2.** For a given starting wavefunction $|\phi\rangle$,
  - (a) and with given g.s. (truncation scheme and) solution, to search in the e.s. CCM for *de-excited states* compatible with the g.s. input; and
  - (b) to invent new truncation schemes.

It is our hope that travelling the various branches of the dual routes above will be sufficient for a universal CCM to be attainable. It is highly probable that Route 2(b) will have to be explored at some length before any real claims to universality can be made in practice. We believe however that further exploration of the easier Route 2(a) may well guide us here, as demonstrated in the previous Section.

To conclude on a different metaphor, we believe that the components of a universal coupled cluster machine have been identified, and that it remains only to assemble it! In any case it is our hope that further work along Route 2(a) along the lines indicated in the previous Section, will provide much information of interest for condensed matter systems, particularly concerning the possibility of new clustered phases.

**References**


12 R.F. Bishop, W. Piechocki and G.A. Stevens (to be published).

   V.C. Aguilera-Navarro, M. de Llano and A. Plastino, KINAM Revista de Fisica 1
   (1979) 441.