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THE COUPLED CLUSTER METHOD: THEORY AND APPLICATIONS TO QUANTUM MANY-BODY AND FIELD-THEORETIC SYSTEMS*

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ABSTRACT

The coupled cluster method (CCM) is one of the most powerful and most successful fully microscopic, *ab initio* formulations available for quantum N-body theory, with N finite or infinite. It has probably been applied to more systems in quantum chemistry, nuclear, condensed matter and other areas of physics, and quantum field theory than any other competing method. In nearly all such cases the numerical results are either the best or among the best available. The CCM can deal with ground- and excited-state energies of closed- and open-shell systems, density matrices and hence other properties, sum rules, and the sub-sum-rules that follow from imbedding linear response theory within it. Extensions exist to deal with systems at nonzero temperature and out of equilibrium. At the formal level it provides an exact mapping of the quantum-mechanical problem onto a classical Hamiltonian phase space where the multiconfigurational canonical classical coordinates have specific cluster and locality properties. In this way it can provide exact hierarchical generalizations of mean-field theory and the random phase approximation. We discuss here both the formalism itself and a selection of its applications.

1. Introduction

Nearly all of physics is many-body physics. This is particularly so at the most fundamental (i.e., the most microscopic) level appropriate to the energy scale of that particular sub-division of the subject under discussion.

There are fields like nuclear, atomic, molecular, and solid-state physics where the fundamentally many-particle aspects of the subject and of its basic objects or systems of interest are immediately apparent. For example, atomic nuclei, atoms, molecules, solids and fluids are manifestly interacting quantum many-body systems. There are other fields like elementary particle physics where it is less immediately apparent that one is also usually dealing with intrinsically many-particle systems rather than only single or few particles. We know, however, that at some level of modelling, even such a 'fundamental' particle as a neutron or proton may be viewed

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* This article is dedicated to J. Dirk Walecka, teacher and friend, on the occasion of his 60th birthday.

as a cloud of mesons surrounding and compressing a smaller bag at its core in which the quarks are confined, or as three quarks interacting via gluons. Thus, our single nucleon has rapidly become a multiparticle problem.

However, at least technically, but also much more deeply and subtly too, the single nucleon is indeed a truly infinite many-body problem since the underlying quantum field theory, namely quantum chromodynamics in this case, intrinsically allows the possibility of the virtual excitation of many particles out of the vacuum. In this sense even the vacuum, the ultimate zero-body problem, becomes endowed with an enormously complex structure due to quantum fluctuations. Indeed, it is no great exaggeration to say that in terms of quantum field theory, the structure of the physical vacuum is the most important many-body problem of all in the field of high-energy particle physics.

It is clear from this last example that quantum field theory may itself be viewed as a branch of quantum many-body theory. Although it is more usual to draw the demarcation line between the two subjects by restricting the quantum many-body problem to systems which obey the non-relativistic Schrödinger quantum mechanics, the overlaps between the two fields are strong. From the modern perspective of fully microscopic, *ab initio* quantum many-body theory, we need a formalism powerful enough to treat, both in principle and in practice, the full range of many-body and field-theoretic systems. We begin by discussing the contenders to play this role.

The most fundamental and more universal tools used nowadays in many-body theory fall into six main classes: time-independent perturbation theory, Green's function or propagator techniques (including parquet or planar theory), variational methods, the method of correlated basis functions, the configuration-interaction method (or the generalized multiparticle shell model), and the coupled cluster method. Each of these methods employs essentially analytical techniques, and is based on a completely microscopic starting point, which is usually the many-body Hamiltonian. A great deal of effort has been expended in each case on the investigation of possible hierarchies of approximations, with the special aim to formulate them in such a way that the results at each order are guaranteed to improve systematically upon those obtained in the preceeding order. It is clearly only within the confines of such an approach that one can be said to possess a rigorous theoretical microscopic understanding of the system. We mention in passing that among the most important of the more heuristic or less theoretically fundamental treatments in the above sense, are the Landau theory of Fermi liquids, the polarisation potential methods of Pines and co-workers, and density functional theory. Finally, sitting as a third paradigm between theory and experiment is the very important class of Monte Carlo or other stochastic simulation techniques, that have grown in importance in recent years with the advent of increasingly powerful computers.

It is my contention that perhaps the only really proven contender that satisfies all of the criteria of being: fully microscopic; widely applicable to a broad spectrum of both finite and extended systems; open to systematic improvement; very accurate (according to the highest precisions attainable by other techniques) in practice; and very widely and deeply tested, is the coupled cluster method (CCM). Certainly, the only other possible candidate in this respect is the correlated basis function method of Feenberg and Clark.

The roots of the CCM lie within nuclear physics[1,2] and the specific need to deal there with the hard-core interaction between two nucleons. Kümmel, one of the co-founders of the method, has recently given[3] a perspective of these historical origins and their relationship to the earlier work in quantum many-body perturbation theory of Brueckner,[4] Goldstone,[5] Hubbard,[6] and Hugenholtz;[7] and to the even earlier work in quantum field theory of Gell-Mann and Low.[8] Most of this latter work has itself been integrated into the now standard textbook of Fetter and Walecka,[9] which has done so much to codify the foundations of modern quantum many-body theory.

In the approximately thirty-five years since its invention, a large panoply of formal developments has taken place under the umbrella title of coupled cluster (CC) theory. The dual aim of the present paper is to give the reader a flavour of what is presently available and to provide a thumbnail sketch of some of the applications of the method so that he or she can appreciate the accuracy and level of description attainable. It is impossible in an article of this size to do full justice either to the method or to those who have developed or applied it. Nevertheless, I will attempt to give sufficient references at the key stages, so that the interested reader may more readily explore the literature. In particular, a considerably fuller and more detailed recent overview article by the same author[10] also covers similar ground and provides a much more exhaustive set of references. A more elementary and pedagogical approach was given earlier by Bishop and Kümmel.[11] Other recommended reviews include those of Refs. [12-23].

In Sect. 2 we attempt an overview of all of the main strands that comprise CC theory, or the CCM, as it exists today. In the space available we can do no more than give the most cursory review of all of the main applications that have been made. We therefore limit ourselves in Sect. 3 to the two illustrative examples of the electron gas (or one-component Coulomb plasma) and pseudoscalar pion-nucleon field theory. In Sect. 4 we give the barest outline of the other main applications made to date.

2. Formal Aspects: Key Elements of the CCM

In its original formulation[1,2] the CCM was invented as a means of parametrizing the exact (pure) ground ket state $|\Psi_0\rangle$ of an interacting N-fermion system at zero temperature, and hence of evaluating its ground-state energy eigenvalue E_0. The parametrization started from a single uncorrelated reference state $|\Phi\rangle$, given as the usual single-particle shell-model (Slater determinant) state formed from an antisymmetrized product of suitably chosen single-particle orbitals. For an extended translationally invariant system this becomes the usual filled Fermi sea of plane-wave states. The multiparticle correlations were then in principle included exactly in terms of an *exponentiated* cluster correlation operator S,

$$|\Psi_0\rangle = e^S|\Phi\rangle; \qquad H|\Psi_0\rangle = E_0|\Psi_0\rangle. \tag{1}$$

This led to the original name of the CCM, the exp(S) method.

The correlation operator S was itself decomposed as a linear superposition of n-body partitions, $S = \sum_{n=1}^{N} S_n$, where S_n describes the configurations formed with respect to this single-reference non-interacting, closed-shell state by the formation of n pairs of single fermions in (particle) orbitals unoccupied in $|\Phi\rangle$ and single vacancies in the corresponding (hole) orbitals occupied in $|\Phi\rangle$. The reason for writing the correlations in exponentiated form in Eq. (1), rather than the linear form, $e^S \rightarrow 1 + F = 1 + \sum_{n=1}^{N} F_n$, typical of the configuration-interaction (CI) method (or generalized shell-model approach), is absolutely fundamental to the CCM. Good heuristic descriptions have been given in earlier pedagogical articles.[3,11] We merely recall here that the exponential form leads to: (i) proper counting of *independent* cluster excitations (e.g., n independent pairs excited from $|\Phi\rangle$ are properly described by the wave function $\frac{1}{n!}S_2^n|\Phi\rangle$); (ii) an automatic incorporation of the important linked cluster theorem of Goldstone;[5] and (iii) hence a correct scaling with particle number N (size-extensivity) of such extensive variables as E_0, in the infinite limit $N \rightarrow \infty$. In some sense the CC exponential ansatz is the quantum-mechanical (i.e., operatorial) analogue of the well-known Ursell-Mayer cluster expansion of classical statistical mechanics.

It is important to realize from the outset that the CCM has now developed far beyond this ground ket-state single-reference level. We attempt in Fig. 1 to give a systematic overview of such other elements of the CCM as now exist, and the relationships between them. In the remainder of this Section we briefly sketch their main ingredients.

The starting point for a CC description is the model (or reference) state $|\Phi\rangle$. Although there is freedom in its choice, the primary requirement on it is that it is a cyclic vector, with respect to which we may define two mutually commuting subalgebras of multiconfigurational creation operators $\{C_I^\dagger\}$ and their Hermitian conjugate destruction operators $\{C_I\}$. Thus, we require that arbitrary ket and bra states within the many-body Hilbert space may be decomposed as the respective linear combinations,

$$|\Psi\rangle = \sum_I \psi_I C_I^\dagger |\Phi\rangle; \qquad \langle\tilde{\Psi}| = \sum_I \tilde{\psi}_I \langle\Phi| C_I. \tag{2}$$

The set-index I labels a general multiparticle cluster configuration with respect to the state $|\Phi\rangle$ in the role of vacuum or reference state.

The choice of $|\Phi\rangle$ clearly depends upon the system under consideration. It is usual for $|\Phi\rangle$ to embody the underlying statistics and other symmetry properties of the system, or its particular phase under consideration, so far as possible. For fermionic systems, the superconducting Bardeen-Cooper-Schrieffer (BCS) state is an alternative choice of $|\Phi\rangle$ to the Slater determinant of single-particle orbitals discussed above. For extended number-conserving bosonic systems a standard choice is the zero-momentum condensate, and for field-theoretic bosonic systems one would usually choose the bare vacuum as model state. Other, less familiar, systems can

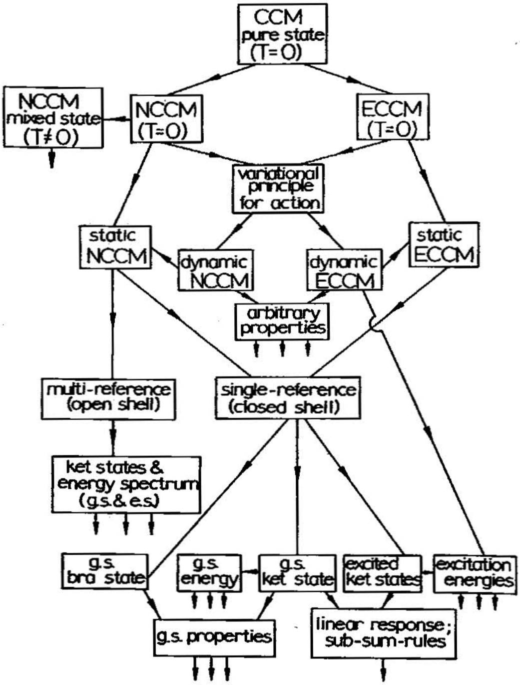

Fig. 1. A schematic outline of the main ingredients of coupled cluster theory, and their inter-relationships.

also be described in the same overall picture. For example, for such spin-$\frac{1}{2}$ magnetic systems as the Heisenberg model defined on a bipartite lattice, $|\Phi\rangle$ may be chosen as the perfectly aligned state in the ferromagnetic regime, or as the classical Néel state in the antiferromagnetic regime, for example. For a further discussion of these very general algebraic foundations of the CCM, the reader is referred to Ref. [19].

With the exact ground ket-state parametrized in the CCM form of Eq. (1), the correlation operator may now be decomposed wholly in terms of creation operators,

$$S = {\sum_I}' s_I C_I^\dagger, \tag{3}$$

where, by definition, the prime on the sum over configurations $\{I\}$ excludes the $I = 0$ term corresponding to the identity operator, $C_0^\dagger \equiv 1$. We thus have the intermediate normalization condition $\langle\Phi|\Psi_0\rangle = \langle\Phi|\Phi\rangle = 1$. The ground-state (g.s.) Schrödinger equation is then rewritten in the similarity-transformed form,

$$(\mathrm{e}^{-S} H \mathrm{e}^{S} - E_0)|\Phi\rangle = 0, \tag{4}$$

which is the hallmark of the CCM. By taking the inner products of Eq. (4) with the complete set of states comprising $|\Phi\rangle$ itself and $\{C_I^\dagger|\Phi\rangle; I \neq 0\}$, we find respectively,

$$E_0 = \langle\Phi|\mathrm{e}^{-S}H\mathrm{e}^{S}|\Phi\rangle = \langle\Phi|H\mathrm{e}^{S}|\Phi\rangle, \tag{5}$$

$$\langle\Phi|C_I\mathrm{e}^{-S}H\mathrm{e}^{S}|\Phi\rangle = 0; \quad I \neq 0. \tag{6}$$

The set of equations (6) represents a coupled set of nonlinear equations for the c-number cluster coefficients $\{s_I\}$, in terms of the solution to which Eq. (5) gives the ground-state energy, $E_0 = E_0[s_I]$. Due to the nested commutator expansion,

$$\mathrm{e}^{-S}H\mathrm{e}^{S} = H + [H,S] + \frac{1}{2!}[[H,S],S] + \cdots, \tag{7}$$

and the fact that all of the individual components of S commute with each other, each element of S in Eq. (3) is linked directly to the Hamiltonian in each of the terms of Eq. (7). Thus, each of the coupled equations of Eq. (6) is of linked-cluster type. Furthermore, the otherwise infinite series of Eq. (7) always terminates in this case after a finite number of terms if, as is usually the case, each term in the second-quantized form of the Hamiltonian contains a finite number of destruction operators, defined with respect to $|\Phi\rangle$. For example, for a system of fermions, say, interacting via two-body forces only, Eq. (7) terminates after the term of fourth order in S.

Equations (6) are therefore of finite order, and need no additional (artificial or approximate) truncation, by contrast to the unitary-transformation equivalent that would arise in a standard variational formulation, in which the bra state $\langle\Psi_0|$ is simply taken as the manifest Hermitian conjugate of $|\Psi_0\rangle$. This feature is important, and leads naturally to the biorthogonal CCM description (rather than the more usual orthogonal one), in which the bra g.s. is parametrized as,

$$\langle\tilde{\Psi}_0| = \langle\Phi|\tilde{S}\mathrm{e}^{-S}; \quad \tilde{S} = 1 + \sum_I{}' \tilde{s}_I C_I; \quad \langle\tilde{\Psi}_0|H = E_0\langle\tilde{\Psi}_0|, \tag{8}$$

in terms of a new correlation operator $\tilde{S}$ composed only of destruction operators with respect to $|\Phi\rangle$. We note that although the manifest Hermiticity is lost, the normalization $\langle\tilde{\Psi}_0|\Psi_0\rangle = 1$ is explicitly imposed. The amplitudes $\{s_I, \tilde{s}_I\}$ now provide a complete description of the g.s. In particular, the g.s. expectation value of an arbitrary operator A may be given as,

$$\bar{A} \equiv \langle\tilde{\Psi}_0|A|\Psi_0\rangle = \langle\Phi|\tilde{S}\mathrm{e}^{-S}A\mathrm{e}^{S}|\Phi\rangle = \bar{A}[s_I, \tilde{s}_I]. \tag{9}$$

The coefficients $\{s_I, \tilde{s}_I\}$ are regarded as being independent parameters, even though formally we have the relation,

$$\langle\Phi|\tilde{S} = \frac{\langle\Phi|\mathrm{e}^{S^\dagger}\mathrm{e}^{S}}{\langle\Phi|\mathrm{e}^{S^\dagger}\mathrm{e}^{S}|\Phi\rangle}. \tag{10}$$

They may themselves be determined variationally by requiring the g.s. expectation value $\bar{H}$ of the Hamiltonian, from Eq. (9), to be stationary with respect to all independent variations. Thus, $\delta\bar{H}/\delta\tilde{s}_I = 0$ gives precisely Eq. (6), whereas $\delta\bar{H}/\delta s_I = 0$ gives the coupled set of equations,

$$\langle\Phi|\tilde{S}\mathrm{e}^{-S}[H, C_I^\dagger]\mathrm{e}^S|\Phi\rangle = 0; \qquad I \neq 0. \tag{11}$$

One may easily verify that Eqs. (6) and (11) are fully equivalent to the bra and ket g.s. Schrödinger equations. The linear set of equations (11) for $\tilde{S}$ may formally be solved as,

$$\langle\Phi|\tilde{S} = \langle\Phi| + \langle\Phi|\mathrm{e}^{-S}H\mathrm{e}^S Q(E_0 - Q\mathrm{e}^{-S}H\mathrm{e}^S Q)^{-1}Q, \tag{12}$$

in terms of the projection operator Q which projects out of the model space spanned by the single reference state $|\Phi\rangle$,

$$Q \equiv 1 - |\Phi\rangle\langle\Phi| = \sum_I{}' C_I^\dagger|\Phi\rangle\langle\Phi|C_I. \tag{13}$$

The expectation value $\bar{A} = \bar{A}[s_I, \tilde{s}_I] \to \bar{A}[s_I]$ then becomes,

$$\begin{aligned}\bar{A} = \bar{A}[s_I] &= \langle\Phi|\mathrm{e}^{-S}A\mathrm{e}^S|\Phi\rangle \\ &+ \langle\Phi|\mathrm{e}^{-S}H\mathrm{e}^S Q(E_0 - Q\mathrm{e}^{-S}H\mathrm{e}^S Q)^{-1}Q\mathrm{e}^{-S}A\mathrm{e}^S|\Phi\rangle.\end{aligned} \tag{14}$$

We note from the CCM Eq. (6) that Eq. (14) reduces to Eq. (5) for the Hamiltonian, $\bar{H}[s_I] = E_0$, at the stationary point. Although this variational formulation does *not* lead to upper bounds for E_0 when S and $\tilde{S}$ are truncated, due to the lack of Hermiticity, it does show rather explicitly that the important Hellmann-Feynman theorem *is* satisfied.

The above static variational principle for the energy expectation value is rather easily generalized to a dynamic variational principle for the action, $\mathcal{A}$,

$$\mathcal{A} \equiv \int_{-\infty}^{\infty} dt\langle\tilde{\Psi}(t)|(i\partial/\partial t - H)|\Psi(t)\rangle. \tag{15}$$

The time-dependent states are now parametrized in the similar CCM form,

$$|\Psi(t)\rangle = \mathrm{e}^{k(t)}\mathrm{e}^{S(t)}|\Phi\rangle; \qquad \langle\tilde{\Psi}(t)| = \mathrm{e}^{-k(t)}\langle\Phi|\tilde{S}(t)\mathrm{e}^{-S(t)}, \tag{16}$$

where $k(t)$ is a necessary c-number scale factor, and otherwise $S = S(t)$ and $\tilde{S} = \tilde{S}(t)$ are parametrized exactly as in Eqs. (3) and (8), but now with time-dependent cluster coefficients $\{s(t), \tilde{s}(t)\}$. The normalization $\langle\tilde{\Psi}(t)|\Psi(t)\rangle = 1$ is still manifestly preserved for all times. Stationarity of $\mathcal{A}$ with respect to all independent variations now readily gives,

$$\frac{\delta A}{\delta\tilde{s}_I} = 0 \iff i\frac{\partial s_I}{\partial t} = \frac{\delta\bar{H}}{\delta\tilde{s}_I}, \tag{17a}$$

$$\frac{\delta A}{\delta s_I} = 0 \iff -i\frac{\partial\tilde{s}_I}{\partial t} = \frac{\delta\bar{H}}{\delta s_I}. \tag{17b}$$

Equations (17a,b) thus show that $\{s_I(t), \tilde{s}_I(t)\}$ are a complete set of canonical coordinates, despite the somewhat asymmetric way they appear in Eqs. (3) and (8). Furthermore, Eqs. (17a,b) show that the CCM parametrization has led in principle to an exact mapping of the original quantum-mechanical many-body/field theory onto the classical mechanics of a set of multiconfigurational classical fields $\{s_I, \tilde{s}_I\}$ with dynamics given by these classical Hamilton's equations. The deep implications of this equivalence are explored elsewhere by the author and his collaborators.[15,19,20,24]

It is clear that by considering small oscillations around the stationary g.s. values, and by performing a linear response analysis of the resulting Eqs. (17a,b), we can put the now classicised problem into normal modes. It is intuitively obvious that the resulting eigenfrequencies and eigenmodes immediately yield the excited-state (e.s.) energy spectrum and wave functions of the original quantum-mechanical problem. A detailed general analysis along these lines has been performed in Ref. [20].

An alternative, time-independent description of excited states has been given by Emrich.[25] Strictly speaking, Eq. (1) describes not only the g.s. but also any state $|\Psi\rangle$ with the same quantum numbers as the g.s. and with nonzero overlap with the model state, $\langle\Phi|\Psi\rangle \neq 0$. The possibility of obtaining multiple solutions to the nonlinear g.s. CCM equations has been discussed in some detail in Ref. [26] for the particular model case of the anharmonic oscillator treated as a single-mode bosonic field theory. For excited states (or, more generally, for states with zero overlap with $|\Psi\rangle$) we construct the respective ket wave functions $\{|\Psi_\lambda\rangle\}$ in the CCM in terms of a set of linear excitation operators $\{X^\lambda\}$,

$$|\Psi_\lambda\rangle = X^\lambda|\Psi_0\rangle = X^\lambda e^S|\Phi\rangle, \tag{18}$$

where X^λ is again decomposed wholly in terms of creation operators with respect to $|\Phi\rangle$,

$$X^\lambda = \sum_I{}' x_I^\lambda C_I^\dagger. \tag{19}$$

Hence, the operators X^λ and S commute. The prime on the sum in Eq. (19) ensures that $\langle\Phi|\Psi_\lambda\rangle = 0$. For extended systems with more than one phase, the so-called g.s. formulation of Eqs. (1) and (3) will generally yield only the lowest state of a given symmetry imposed implicitly by the particular choice of $|\Phi\rangle$. Indeed, phase transitions may often be detected within this CCM description by observing (for fixed $|\Phi\rangle$) the onset of "excited" states of negative excitation energy from Eqs. (18)-(19), as some parameter characterizing the system is varied beyond some critical value. This point has been discussed more fully elsewhere.[27]

The e.s. Schrödinger equation,

$$H|\Psi_\lambda\rangle = E_\lambda|\Psi_\lambda\rangle \equiv (E_0 + \epsilon_\lambda)|\Psi_\lambda\rangle, \tag{20}$$

may be combined with its g.s. counterpart to derive the equivalent CCM eigenvalue equations,

$$e^{-S}[H, X^\lambda]e^S|\Phi\rangle = \epsilon_\lambda X^\lambda|\Phi\rangle, \tag{21a}$$

$$(\mathrm{e}^{-S}H\mathrm{e}^{S} - E_0)X^{\lambda}|\Phi\rangle = \epsilon_{\lambda}X^{\lambda}|\Phi\rangle, \tag{21b}$$

for the excitation energy $\epsilon_\lambda \equiv (E_\lambda - E_0)$ directly. We may now simply write down a coupled set of linear eigenvalue equations for the e.s. configuration coefficients $\{x_I^\lambda\}$ by taking the inner products of Eq. (21a) or Eq. (21b) with each member of the set $\{C_I^\dagger|\Phi\rangle; I \neq 0\}$. It is clear that, formally, the excitation energies $\{\epsilon_\lambda\}$, are simply the eigenvalues obtained by diagonalizing the same matrix $Q(\mathrm{e}^{-S}H\mathrm{e}^{S} - E_0)Q$ as needs formally to be inverted to obtain $\tilde{S}$, as in Eq. (12). We also note that the left-hand side of Eq. (21a) again has the form of a similarity transform, which may be expanded by analogy with Eq. (7). In this way we observe that the e.s. CCM equations may rather simply be derived from their g.s. counterparts by replacing each multinomial term in the coefficients $\{s_I\}$ arising from the expansion of the left-hand side of Eq. (4) with a corresponding set of terms in which each single coefficient s_J, is replaced one at a time by the corresponding factor x_J^λ, and where the zeroth-order (inhomogeneous) terms in $\{s_I\}$ are dropped.

In order to implement any of the above CCM schemes in practice, one needs to approximate. This is done by restricting the otherwise complete set of configuration indices $\{I\}$ for the various cluster configuration operators (e.g., $S, \tilde{S}, X^\lambda$) to some particular finite or infinite subset, according to some well-defined hierarchical approximation scheme. There are clearly many ways of doing this. One of the simplest is the so-called SUB(n) scheme for either the static formulation of Eqs. (1), (3) and (8) or the dynamic formulation of Eq. (16). Here, the configurations $\{s_I, \tilde{s}_I\}$ which describe clusters of more than n particles (or particle-hole pairs in the case of Fermi systems) are set to zero. An extension for the static e.s. formalism is the so-called SUB(m,n) scheme in which all configurations $\{x_I^\lambda\}$ and $\{s_I\}$ which describe clusters of more than m and n particles (or particle-hole pairs) respectively are set to zero. All remaining equations, derived as described previously, for the configurations retained, are then solved without further approximation.

It should be clear that in the SUB(m,n) scheme, the excitation energies $\{\epsilon_\lambda\}$ are equivalently obtained by diagonalizing the operator $Q(\mathrm{e}^{-S}H\mathrm{e}^{S} - E_0)Q$, where S is the SUB(n)-truncated CCM g.s. correlation operator, within the subspace of multiconfigurational states defined by the truncation index m. The freedom in choosing m and n independently allows considerable flexibility in implementation. Further work in this connection[18] has shown that by also imbedding the theory of linear response within the CCM, each of the usual energy-weighted-moment sum rules for the dynamic (liquid) structure function can be exactly decomposed into an infinite cluster hierarchy of sub-sum-rules. It is interesting to note that by making the simple approximation that the lowest members of the CCM sub-sum-rules are exhausted by a single (collective or "giant resonance") state, we regain the important Bijl-Feynman relation for the excitation spectrum in terms of the static structure function.

For the static g.s. CCM formalism, the remaining (suitably truncated) equations for the cluster configuration coefficients $\{s_I\}$ may be arranged in such a way that upon iteration they yield precisely the well-known time-ordered Goldstone diagrams of time-independent many-body perturbation theory. The interested reader is referred to the literature[12,13,16] for further details. A rather full derivation and discussion of the extremely rich SUB(2) approximation for infinite homogeneous media is given in Ref. [12], for example. It should be clear to the reader that the cluster coefficients $\{s_I, \tilde{s}_I\}$ may also be viewed as generalized multiparticle mean fields or as generalized collective coordinates. In this way, hierarchical approximation schemes for the static and dynamic CCM formalisms respectively provide equivalent generalizations of mean-field theory[19] and the random phase approximation.[20] Finally, we note that other approximation schemes, apart from the SUB(m, n) scheme above, have been devised for specific systems. For example, in the case of quantum spin lattice problems, quite different localized approximation schemes have also been very successfully employed.[28]

Everything that we have described so far within the CCM is nowadays described as the normal coupled cluster method (NCCM), to distinguish it from an extended version (or ECCM). Briefly, although out of the complete set of coordinates $\{s_I, \tilde{s}_I\}$ which, in principle, fully parametrize our quantum many-body system, the coefficients $\{s_I\}$ are completely linked, the bra-state coefficients $\{\tilde{s}_I\}$ are unlinked. While this has no effect at all on the linked nature of arbitrary expectation values $\bar{A}$ in Eq. (9), for many purposes it is useful (if not vital) to have *all* of the cluster configuration coefficients linked. This is precisely what is achieved in the ECCM,[15] a complete description of which would now take us too far afield. We merely remark here that at the formal level, the ECCM has a double exponential structure which, in turn, leads to a double similarity transform structure and a double-linking structure to its diagrams.

By contrast with both the configuration-interaction method (where neither bra- nor ket-state cluster coefficients are fully linked) and the NCCM (where only half the coefficients are linked), all of the basic ECCM aplitudes are linked-cluster quantities with well-defined diagrammatic representations.[15] In turn, therefore, they all obey the important cluster property, namely that they become asymptotically zero as any subset of particles described by the amplitude becomes far removed in real space from the remainder. The ECCM also provides an equivalent classicisation mapping to that provided by the NCCM via Eqs. (17a,b), but now *all* of the classical fields or amplitudes are local (or, better, multi-local) in the sense of obeying the cluster property. We note here only that the ECCM is, to the best of our knowledge, unique as a formulation of quantum many-body/field theory in which *every* fundamental amplitude exactly obeys the cluster property at all reasonable levels of approximation. It is clear that only such formulations have the possibility to describe both the local properties of many-body systems and such global properties as their phase transitions, states of topological excitation or deformation, spontaneous symmetry breaking, and general nonequilibrium behaviour. We indicate schematically in Fig. 2 the overall structure of the ECCM, and refer the reader to the literature[15,19,20,22–24] for further details.

Finally, to complete our discussion of Fig. 1, we note firstly that independent extensions of the previous NCCM analysis of pure states to deal with mixed

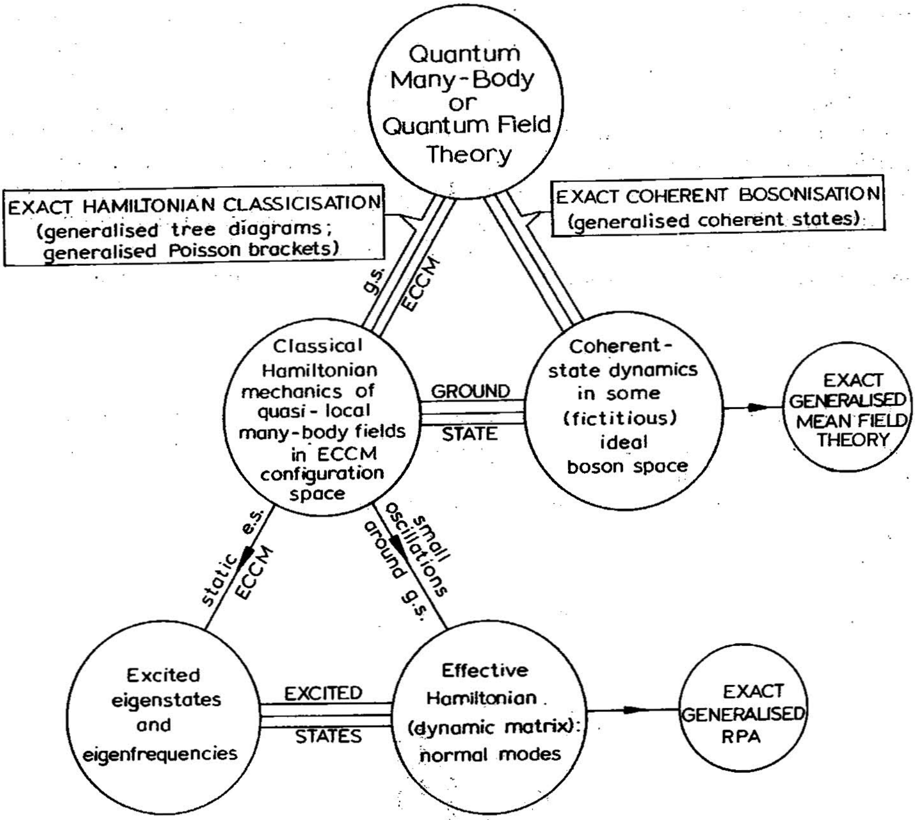

Fig. 2. A schematic representation of the hierarchical structure and general features of the extended coupled cluster method (ECCM) of quantum many-body and quantum field theory.

states, and hence systems at nonzero temperatures, have also been given both within the stationary formalism in terms of the Bloch equation for the statistical density operator,[29] and within an imaginary-time formalism for the partition function.[30] Secondly, we note that just as the single-reference version of the NCCM described above incorporates the Goldstone linked cluster theorem[5] for the energy in the context of nondegenerate perturbation theory, so a multi-reference version of the NCCM also exists,[31] which incorporates the linked valence expansion of Brandow[32] in the context of degenerate many-body perturbation theory and its diagrammatic expression in terms of so-called folded diagrams.

The essential ingredients of the multi-reference formalism are indicated schematically in Fig. 3. Thus, we start with a closed-shell system of N particles, whose CCM single-reference model state is $|\Phi\rangle \equiv |\Phi_N\rangle$, and whose exact g.s. energy is $E_0 \rightarrow E_0^N$. We now add valence particles (or holes) one at a time. The basic idea is to keep the closed shell as a starting wave function, and to incorporate into it the extra correlations arising from the valence particles. If we denote the single-particle creation operators as $\{a_\alpha^\dagger\}$, we may distinguish three sorts of single-particle states, namely: (i) orbitals occupied in $|\Phi_N\rangle$ (labelled $\alpha \rightarrow \mu, \nu, \ldots$); (ii) valence orbitals (labelled $\alpha \rightarrow i, j, \ldots$) partially occupied by the valence particles outside the core; and (iii) the remaining "unoccupied" orbitals (labelled $\alpha \rightarrow \rho, \sigma, \ldots$). The multi-reference CCM ansatz for the exact $(N+1)$-particle states is given as,

$$|\Psi_{N+1}^\alpha\rangle = \sum_i^{\mathcal{V}} \mathrm{e}^S[1 + F^{(1)}]a_i^\dagger|\Phi_N\rangle C_i^\alpha, \tag{22}$$

where S is assumed known from the N-body "closed-shell" calculation, and where the sum on i runs over the set $\mathcal{V}$ of valence orbitals considered as degenerate or quasidegenerate. Thus, the states $\{a_i^\dagger|\Phi_N\rangle;\ i \in \mathcal{V}\}$ form a set of multi-reference $(N+1)$-body Slater determinants for the low-lying states $\{\alpha\}$ which we wish to construct.

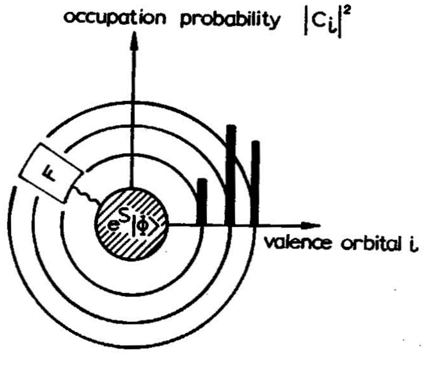

Fig. 3. A schematic representation of the main ingredients of the multi-reference coupled cluster parametrization of the ket-state wave functions of an open-shell system.

Whereas, the coefficients $\{C_i^\alpha\}$ determine the mixture of uncorrelated states in the multi-reference model state, the operator $F^{(1)}$ describes the dressing of the bare valence particle by its interactions with the core. It may be decomposed as,

$$F^{(1)} = \sum_{n=1}^{N+1} F_n^{(1)}, \tag{23}$$

where, for example, $F_1^{(1)}$ describes the one-body (Hartree-Fock) part of the valence problem,

$$F_1^{(1)} = \sum_{\rho} \sum_{i}^{\mathcal{V}} \langle \rho | F_1^{(1)} | i \rangle a_\rho^\dagger a_i, \tag{24}$$

and $F_2^{(1)}$ describes the "core polarization" terms which arise from the correlations between the valence particle and any one core particle,

$$F_2^{(1)} = \frac{1}{2} \sum_{\eta_1,\eta_2} \sum_{\nu} \sum_{i}^{\mathcal{V}} \langle \eta_1 \eta_2 | F_2^{(1)} | i\nu \rangle_A a_{\eta_1}^\dagger a_{\eta_2}^\dagger a_\nu a_i, \tag{25}$$

where the labels η_1 and η_2 indicate any extra-core state (i.e., valence or "unoccupied"). We note that the CCM ansatz of Eq. (22) is completely general provided only that, as in the single-reference counterpart of Eq. (1), the states $|\Psi_{N+1}^\alpha\rangle$ do not have zero overlap with all of the wave functions $\{a_i^\dagger|\Phi_N\rangle; i \in \mathcal{V}\}$ in the model space.

The comparable ansatz for the two valence-particle $(N+2)$-body wave function is,

$$|\Psi_{N+2}^\beta\rangle = \sum_{i,j}^{\mathcal{V}} \mathrm{e}^S [1 + F^{(1)} + \frac{1}{2} : F^{(1)^2} : + F^{(2)}] a_i^\dagger a_j^\dagger |\Phi_N\rangle C_{ij}^\beta, \tag{26}$$

where the factor of $1/2$ in the quadratic term describing two "dressed" but uncorrelated valence particles prevents us from counting each excitation twice. This term is also normal-ordered so as to avoid contractions (or links) between them, which are more properly contained in the genuine two-valence-particle-plus-core correlation operator $F^{(2)}$,

$$F^{(2)} = \sum_{n=2}^{N+2} F_n^{(2)}. \tag{27}$$

If we proceed further in this fashion to add more valence particles outside the core, we rapidly arrive at the normal-ordered exponential ansatz first written down explicitly by Lindgren,[33] although the formulation of Ey[31] is equivalent.

Insertion of Eqs. (21) and (25) into the respective $(N+1)$-body and $(N+2)$-body Schrödinger equations, and premultiplication as usual by the factor e^{-S}, leads readily to equations for the energy eigenvalues E_α^{N+1} and E_β^{N+2}. Suitable projections onto the model space thus lead to secular equations for the coefficients C_i^α and C_{ij}^β. It is easily shown[13,16,31] that these may be represented as generalized eigenvalue equations for fully-linked one-and two-body effective Hamiltonians respectively (which yield the folded diagrams of degenerate perturbation theory), with eigenvalues equal to the respective excitation energies, e.g., $\epsilon_\alpha \equiv E_\alpha^{N+1} - E_0^N$ for the single-valence case. Similarly, by projecting out of the model space onto "unoccupied" states, we may derive equations which determine the matrix elements of the operators $F^{(1)}$ and $F^{(2)}$. The interested reader is referred to the literature cited above for further details.

In the remainder of this paper we now indicate some of the main applications of the CCM techniques described in this Section and summarized diagramatically in Fig. 1.

3. Illustrative Examples of CC Applications

3.1. The Electron Gas

The electron gas (or "jellium")[9] was originally invented to model the electrons in a metal, in a simplified form in which the ionic lattice is replaced by a uniform positive charge as an inert neutralizing background. The two-body potential is otherwise pure Coulombic, and is given in momentum-space representation as,

$$V(\mathbf{q}) = \frac{4\pi e^2}{\Omega q^2}(1 - \delta_{\mathbf{q}0}), \tag{28}$$

where Ω is the normalization volume. More generally, a system of N identical particles (bosons or fermions), of mass m and charge e each, interacting via the two-body potential of Eq. (28), is denoted as the one-component Coulomb plasma. The number density, $\rho \equiv N/\Omega$, may be expressed as,

$$\rho = (4\pi r_s^3 a_0^3/3)^{-1} = k_F^3/3\pi^2, \tag{29}$$

in terms of either the only independent dimensionless coupling constant, $r_s \equiv r_0/a_0$, which characterizes the system, namely the average interparticle spacing, r_0, in units of the Bohr radius, $a_0 \equiv \hbar^2/me^2$, or a (what is for bosons purely fictitious) wave number k_F applicable to an unpolarized spin-$\frac{1}{2}$ system. (Henceforth, we use units such that $\hbar = 1$.) Equation (29) implies the relation,

$$k_F a_0 = (\alpha r_s)^{-1}; \quad \alpha \equiv (9\pi/4)^{-1/3}. \tag{30}$$

We also define the g.s. energy per particle in Rydberg units as,

$$E_0/N = \epsilon(e^2/2a_0), \tag{31}$$

and, as necessary, scale momentum variables in units of k_F defined in Eq. (28), as $\mathbf{q} = k_F\mathbf{x}$.

The one-component Couloumb plasmas are interesting because they exhibit a phase transition between the high-density (weak-coupling, $r_s \to 0$) plasma limit and the low-density (strong-coupling, $r_s \to \infty$) limit of a Wigner crystal. They are also analytically clean in that they contain only one dimensionless coupling parameter, r_s. The quantum statistics play a crucial role at high and intermediate densities, but their importance vanishes in the essentially classical low-density limit.

Furthermore, these systems are highly nontrivial for all values of r_s due to the long-range (r^{-1}) nature of the Coulomb potential.

We consider first the CCM treatment of the algebraically simpler bosonic plasma. As reference state we take the zero-momentum condensate,

$$|\Phi\rangle = (N!)^{-1/2}(b_0^\dagger)^N|0\rangle, \tag{32}$$

where $|0\rangle$ is the vacuum state, and $\{b_\alpha^\dagger\}$ are a complete set of single-boson creation operators. In the plane-wave momentum-eigenstate representation, $\alpha \to 0$ labels the sole "occupied" (and hence hole) state, and $\alpha \to \mathbf{q}(\neq 0)$ labels the "unoccupied" particle states. The cluster correlation operator of Eqs. (1) and (3) takes the explicit form,

$$S = \sum_{n=2}^{N} S_n; \quad S_n = \frac{1}{n!}\sum_{\mathbf{q}_1\cdots\mathbf{q}_n} S_n(\mathbf{q}_1,\ldots,\mathbf{q}_n) b_{\mathbf{q}_1}^\dagger\cdots b_{\mathbf{q}_n}^\dagger (N^{-1/2}b_0)^n, \tag{33}$$

where the matrix elements in Eq. (33) are subject to the condition $\sum_{i=1}^{n}\mathbf{q}_i = 0$, which arises from the assumption that the $N \to \infty$ ground state is that of a homogeneous (translationally-invariant) phase.

In the present case where the interaction potential is of local two-body type, and with the added constraint from Eq. (28) that $V(\mathbf{q}=0) = 0$, one may show that the *exact* two-body equation for $S_2(q) \equiv S_2(\mathbf{q},-\mathbf{q})$ becomes

$$\begin{aligned}&\frac{q^2}{m}S_2(q) + T_{\text{RPA}} + T_{\text{CP}} + T_{\text{LAD}} + \Omega\int\frac{d^3q'}{(2\pi)^3}V(q') \\ &\quad\times\left[2N^{1/2}S_3(\mathbf{q},\mathbf{q}',-\mathbf{q}-\mathbf{q}') + \frac{1}{2}NS_4(\mathbf{q},-\mathbf{q},\mathbf{q}',-\mathbf{q}')\right] = 0,\end{aligned} \tag{34}$$

in the thermodynamic limit where $N \to \infty$ at fixed ρ, and where

$$T_{\text{RPA}} = NV(q)[1+S_2(q)]^2, \tag{35a}$$

$$T_{\text{CP}} = -\frac{4E_0}{N}S_2(q), \tag{35b}$$

$$T_{\text{LAD}} = \Omega\int\frac{d^3q'}{(2\pi)^3}V(\mathbf{q}-\mathbf{q}')S_2(q'), \tag{35c}$$

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

$$\frac{E_0}{N} = \frac{1}{2}\Omega\int\frac{d^3q}{(2\pi)^3}V(q)S_2(q). \tag{36}$$

The SUB(2) approximation is obtained from Eq. (34) by setting S_3 and S_4 to zero. The remaining four terms represent respectively: (i) the kinetic energy

(KE) contribution; (ii) the terms that together with KE generate precisely the random phase approximation (RPA); (iii) the terms that generate the self-consistent energy insertions on the hole lines, namely the condensate potential (CP) terms; and (iv) the terms that generate the two-boson ladder (LAD) diagrams for repeated scattering of a pair from out of the condensate. When fully expressed in terms of dimensionless variables, the SUB(2) equation for the bosonic Coulomb plasma becomes,

$$x^2 S_2(x) + \frac{4\alpha r_s}{3\pi x^2}[1+S_2(x)]^2 - 2(\alpha r_s)^2 \epsilon S_2(x) + \frac{\alpha r_s}{\pi x}\int_0^\infty dx' x' \ln\left|\frac{x'+x}{x'-x}\right| S_2(x') = 0, \tag{37}$$

$$\epsilon = \frac{2}{\pi \alpha r_s}\int_0^\infty dx S_2(x). \tag{38}$$

Although the nonlinear equation (37) is readily solved numerically, it is more instructive to examine its high- and low-density limits. In the high-density limit, it is trivial to show that,

$$\epsilon \underset{r_s \to 0}{\longrightarrow} Q r_s^{-3/4} + R, \tag{39}$$

and, furthermore, that only the KE and RPA terms contribute to leading order, to give the well-known exact result,

$$Q = -\frac{16}{5}\left(\frac{3}{\pi^2}\right)^{1/4} \frac{\Gamma(3/4)}{\Gamma(1/4)} \approx -0.8031, \tag{40}$$

first obtained by Foldy.[34] The CP and LAD terms also contribute to next order to give a SUB(2) value for the constant R of $16/9\pi$. Inspection of Eqs.(34)-(35) shows that the coupling terms to S_3 and S_4 also contribute to the constant R (although not to Q). A careful and detailed calculation[35] including these terms leads to the value $R \approx 0.0280$, and an intricate rearrangement of terms shows that this result is identical to the first correct result reported, namely that of Brueckner.[36] It is also worth noting that, by contrast with most competing approximations, each term generated by the SUB(2) approximation is finite and no (cancellations between) spurious logarithmic singularities occur. This point illustrates the more general feature of the CCM that terms which tend to cancel one another are automatically grouped together and/or are never split apart.

In the opposite strong-coupling ($r_s \to \infty$) limit, one may not expect the above SUB(2) approximation to be at all accurate, since one imagines that n-body clusters with $n \gg 2$ are now important. Indeed, we expect the system to Wigner crystallize below some critical density, and such a crystal phase is an archetype of a situation where N-body correlations dominate. Furthermore, the translational-invariance symmetry of $|\Phi\rangle$ and the Hamiltonian is also spontaneously broken in the crystalline phase. However, in the SUB(2) approximation we find the result,

$$\epsilon \underset{r_s \to \infty}{\longrightarrow} -Ar_s^{-1} + Br_s^{-3/2} + O(r_s^{-2}), \tag{41}$$

typical of the solid phase, even though the numerical values of the coefficients A and B are not precisely those of the actual b.c.c. lattice. A more detailed discussion of this surprising result has been given elsewhere,[35] and we do not pursue it further here.

Instead, we turn next to the fermionic Coulomb plasma, and restrict ourselves to the unpolarized spin-$\frac{1}{2}$ electron gas. The analogue of Eq. (32) for a translationally-invariant system is now the usual filled Fermi sea with Fermi wave number k_F. In the thermodynamic limit the fermionic SUB(2) analogue of Eq. (37) is a nonlinear integral equation in three three-momentum variables for the antisymmetrized matrix elements,

$$S_2^{\sigma_1\sigma_2}(\mathbf{k}_1, \mathbf{k}_2; \mathbf{q}) \equiv \langle \mathbf{k}_1 + \mathbf{q}, \sigma_1; \mathbf{k}_2 - \mathbf{q}, \sigma_2 | S_2 | \mathbf{k}_1\sigma_1; \mathbf{k}_2\sigma_2 \rangle_A, \tag{42}$$

which depend not only on a momentum transfer $\mathbf{q}$ as for bosons, but also on the two hole-state momenta $\mathbf{k}_1$ and $\mathbf{k}_2$ inside the Fermi sphere, as well as the spin-projection indices $\sigma_1, \sigma_2 (= \pm\frac{1}{2})$. The corresponding SUB(2) equation is thus much more complex than Eq. (37). It has been described fully elsewhere.[12]

Once again, it can be shown[12] that in the weak-coupling ($r_s \to 0$) plasma regime, the SUB(2) equation reduces to a leading contribution which is the complete analogue of the KE and RPA terms of Eq. (34). The RPA[9] is well known to give the exact leading high-density contribution to the correlation energy, ϵ_c, where

$$\epsilon \equiv \epsilon_0 + \epsilon_c; \qquad \langle \Phi_F | H | \Phi_F \rangle \equiv N\epsilon_0 (e^2/2a_0). \tag{43}$$

The corresponding nonlinear RPA equation for S_2 has been solved exactly,[12] and the leading (logarithmic) contribution to ϵ_c at high densities has been verified.

In the intermediate-coupling regime ($1 \leq r_s \leq 5$) of metallic densities, we no longer expect the RPA to suffice. Thus, apart from neglecting (i) the simple exchange terms needed to antisymmetrize RPA, we have omitted from even the SUB(2) approximation: (ii) all combined particle-particle and hole-hole ladder terms, some at least of which are important for describing correctly the 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. Since the full SUB(2) equation is so technically complicated, a "state-averaging" approximation method was introduced[35] in order to proceed systematically beyond RPA. It was motivated by analogy with the mathematically much simpler Bose equations (34). The basic approximation is to average inside the Fermi sea over the hole momenta $\mathbf{k}_1$ and $\mathbf{k}_2$

in $S_2(\mathbf{k}_1, \mathbf{k}_2; \mathbf{q})$. However, in performing this averaging the very important Pauli exclusion principle is preserved by requiring that the particle momenta $(\mathbf{k}_1 + \mathbf{q})$ and $(\mathbf{k}_2 - \mathbf{q})$ simultaneously lie outside the Fermi sea. In this way the exact $S_2(\mathbf{k}_1, \mathbf{k}_2; \mathbf{q})$ is replaced by an approximate state-averaged $\overline{S}_2(q)$. The precise details are described in Ref. [35]. The approximation was tested on the RPA where it was shown to be exact in the high-density limit ($r_s \to 0$), and to give results better than 2% accuracy at *all* densities.

The same state-averaging procedure was then implemented on the full SUB(2) equation and, furthermore, with the additional inclusion of some of the more important contributions for the coupling terms to S_3 and S_4. Results from such calculations were first presented by Bishop and Lührmann.[35] They were later repeated by Emrich and Zabolitzky.[37] These latter authors also avoided the use of several additional minor approximations made by the former, and their CCM results are shown in Table 1, where they are labelled CC(4) to indicate that they include at least part of the contributions from triple and quadruple excitations.

Table 1. Correlation energy per particle (in milli-Rydbergs) of the unpolarized electron gas, for various values of the dimensionless coupling constant, r_s.

r_s	$\to 0$	1	2	3	4	5	6	10	20
RPA	$62.2 \ln r_s$	−158	−124	−106	−93.6	−84.9	−78.2	−61.3	−42.8
CC4[a]	$62.2 \ln r_s$	−122	−90.4	−73.8	−63.4	−56.0	−50.5	−37.0	−23.6
GFMC[b]	$[62.2 \ln r_s]$	−121	−90.2	[−73.8]	[−63.6]	−56.3	[−50.7]	−37.22	−23.00
FHNC[c]	$57.0 \ln r_s$	−114	−85.9	−71.0	−61.2	−54.1	—	−35.5	−21.8
VS[d]	—	−130	−98	−81	−70	−62	—	—	—

[a] CCM result of Emrich and Zabolitzky[37]

[b] Green's function Monte Carlo result of Ceperley and Alder, with the results in brackets obtained by the interpolation procedure of Vosko et al.[39]

[c] Results of a Fermi hypernetted chain type of variational calculation of Zabolitzky[38]

[d] Results of a phenomenological approach of Vashishta and Singwi[40]

We compare the CCM results in Table 1 with the Green's function Monte Carlo results[38] which come from an essentially exact (apart from statistical errors) stochastic simulation of the many-electron Schrödinger equation. We also compare with representative results from the best of the other available calculations, including a variational calculation of Zabolitzky,[39] and a more phenomenological calculation of Vashishta and Singwi.[40] It is clear that over the entire metallic density regime the CCM results are extraordinarily accurate. Indeed, we know of no better microscopic description of the electron gas at these densities. Since the electron gas is still perhaps one of the most well-studied of all quantum many-body problems, we believe that these results amply demonstrate the power and accuracy of the CCM.

3.2. Pseudoscalar Pion-Nucleon Field Theory

A rather different application of the CCM techniques described in Sect. 2 is provided by the standard (3+1)-dimensional model of pions and nucleons interacting via an isospin-invariant pseudosalar coupling. The model is described in terms of the Hamiltonian density,

$$\mathcal{H} = \mathcal{H}_0 + \mathcal{H}_{\rm int},$$

$$\mathcal{H}_0 = \mathcal{H}_0(\mathbf{x}) = \frac{1}{2}[\Pi_t^\dagger \Pi_t + \nabla\Phi_t^\dagger \cdot \nabla\Phi_t + m_0^2 \Phi_t^\dagger \Phi_t] + \overline{\Psi}_{t'}(-i\gamma\cdot\nabla + M_0)\Psi_{t'}, \tag{44}$$

$$\mathcal{H}_{\rm int}(\mathbf{x}) = -ig\int d^3x' F(\mathbf{x}-\mathbf{x}')\overline{\Psi}_{t'}(\mathbf{x})\gamma_5\tau_t\Psi_{t'}(\mathbf{x})\Phi_t(\mathbf{x}'),$$

where $\Phi_t = \Phi_t(\mathbf{x})$ and $\Pi_t = \Pi_t(\mathbf{x})$ are respectively the (bosonic) pion field operator and its conjugate momentum density operator, and $\Psi_{t'}(\mathbf{x})$ and $\overline{\Psi}_{t'}(\mathbf{x})$ are respectively the (fermionic) four-component Dirac nucleon field operator and its adjoint. The matrices γ and γ_5 are the usual 4×4 Dirac matrices; the three matrices τ_t are the usual 2×2 Pauli isospin matrices; and the summation convention is implied over the repeated isospin indices t' for the (isospin-$\frac{1}{2}$) nucleon and t for the (isospin-1) pion. The form factor $F(\mathbf{x})$ is necessary to renormalize the pion-nucleon vertex. It is taken to have the usual Yukawa form, given by its Fourier transform in momentum space as,

$$F(\mathbf{q}) = \frac{\lambda^2 - m_0^2}{\lambda^2 + q^2}, \tag{45}$$

where λ is a high-momentum (or, equivalently, small-distance) cutoff parameter. Finally, the mass parameters m_0 and M_0 are the *bare* pion and nucleon masses, respectively.

A CCM calculation for this system has been performed[41] within the multi-reference ("open-shell") formulation described in Sect.2. The *physical* vacuum $|\Psi_0\rangle$ is first written in terms of the *bare* vacuum $|\Phi\rangle$ exactly as in Eq. (1), in terms of a cluster correlation operator S which is now expanded as a double sum,

$$S = \sum_{m,n=1}^{\infty} S_{m,n}, \tag{46}$$

in terms of the number m of pions and the number n of nucleon-antinucleon pairs virtually excited. Secondly, the (physical) one-nucleon state is treated exactly as in the one-valence parametrization of Eq. (22); and, thirdly, the two-nucleon state is treated as in the two-valence parametrization of Eq. (26). The operators $F^{(1)}$ and $F^{(2)}$ are also decomposed as in Eq. (46).

Such a multi-reference CCM calculation has been performed by Hasberg and Kümmel,[41] in which they retained the partitions $S_{0,1}, S_{1,1}, F^{(1)}_{1,0}$ (and $F^{(1)}_{2,0}, F^{(1)}_{0,1}$ and $F^{(1)}_{1,1}$ in low order). The results clearly depend upon the free parameters M_0, g, and

λ. In principle, they also depend on m_0, but it turns out that the pion self-energy is actually a higher-order effect than the above approximations used, and hence m_0 is set to the physical (experimental) pion mass of about 139 MeV. The one-nucleon calculation was then used to fit the bare mass M_0 so as to give a CC outcome for the physical nucleon mass equal to its experimental value, 940 MeV, for a particular choice of λ and g. Finally, with all parameters thus fixed, the two-nucleon (deuteron) binding energy was predicted. For example, with the pion-nucleon coupling constant set at the physical ("experimental") value, $g^2/4\pi = 14.4$, and with $\lambda = 1000, 1300$, and 1500 MeV respectively, bare nucleon masses of $M_0 = 726$, 664, and 651 MeV respectively give a physical nucleon mass equal to 940 MeV in each case, and a deuteron binding energy of 9.4, 10.5, and 10.8 MeV respectively. It is particularly gratifying to note that the dependence on λ is very weak. Alternatively, it was found that to get the deuteron binding energy in the above calculation to emerge at the experimental value of 2.22 MeV, using a cutoff parameter $\lambda = 1000$ MeV, for example, required a bare nucleon mass $M_0 = 771$ MeV and a value for $g^2/4\pi$ reduced by only a factor 1.28 from the above physical value.

The convergence obtained in these pioneering calculations is most impressive, and indicates that CCM techniques which have been widely used in, for example, quantum chemisry and nuclear physics to treat atoms, molecules and nuclei, can also find valuable applications in quantum field theory.

4. Other Applications of the CCM

Many other equally impressive applications of the CCM have been made. In an article of this size we can do little other than list them below. For further details the interested reader is referred to the literature already cited, in particular Ref. [10] and the references quoted therein.

• *Nuclear physics:* Many applications of the CCM have been made for finite nuclei,[13,16] both for such closed-shell nuclei as ^{4}He, ^{16}O and ^{40}Ca, and such open-shell nuclei as ^{15}N and ^{17}O, and ^{14}C, ^{18}O and ^{18}F that can be obtained from them by the addition of one or two valence particles or holes. Calculated quantities include g.s. energies, density distributions, elastic-scattering electron form factors, and excitation spectra. What are probably still the best perturbative-type calculations of nuclear matter,[42] including three-body and (the most important) four-body cluster terms, have also been performed within the CCM framework. By contrast with most other calculations being done even now (especially for open-shell nuclei), essentially all of these CCM calculations in nuclear physics are demonstrably converged.

• *Quantum chemistry:* The very high accuracy required nowadays for the calculation of parity violation in atoms, as well as for the calculation of molecular energy differences of chemical significance, calls for extreme accuracy in the solution of the electron correlation problem. The success demonstrated above for the electron gas clearly demonstrates that the CCM is excellently suited for such use. Indeed, it is now widely recognized as the method of first choice in terms of power and accuracy, for calculations on, for example, ionization potentials, electron affinities, Auger spectroscopy, excitation energies and energy gradients (for use, for example, in searching potential energy surfaces to predict vibrational spectra or to locate transition states in decomposition reactions). A huge number of atoms and molecules (including, e.g., LiH, H_2O, GaAs, benzene, etc.) has been studied, and state-of-the art calculations are now done on molecules with up to 80 active electrons.[14,17,21,43]

• *Model many-body problems:* Examples here include: (i) the Lipkin-Meshkov-Glick SU(2) quasispin model of the spherical to deformed shape transition in the rare-earth nuclei under rotation; (ii) the exactly integrable one-dimensional Lieb model of bosons interacting via pairwise repulsive delta-function potentials; and (iii) the polaron problem.

• *Quantum field theory:* Apart from the model outlined in Sect. 3.2, other examples which have been studied by CCM techniques include: (i) anharmonic oscillators treated as a single-mode (0+1)-dimensional bosonic field theory; (ii) Φ^4 bosonic field theory in (1+1) and (2+1) dimensions; and (iii) lattice gauge field theories, e.g., Z_2 and U(1) (i.e., lattice quantum electrodynamics).

• *Quantum spin chain and lattice models:* Recent successful applications of the CCM have been made to both the solid phases of ^{3}He and various models exhibiting antiferromagnetism.[28] The latter includes the Heisenberg model on a two-dimensional square lattice, which is believed to be of relevance to the (undoped) ceramic cuprate high-temperature superconductors.

• *Quantum fluid mechanics:* A recent application of the ECCM[44] has been made to the strongly-interacting condensed Bose fluid at zero temperature where, *inter alia*, a hierarchy of exact local balance equations (for number conservation, momentum conservation, energy conservation, etc.) is derived microscopically. These are precisely the quantum-mechanical macroscopic laws of hydrodynamics for the system. Furthermore, the well-known Gross-Pitaevskii approximation[9] for this system is regained at the lowest level of implementation of the CCM, namely SUB(1).

• *Charged impurity in a polarizable medium:* The technique of allowing a low-energy positron to annihilate inside metals, alloys, and other forms of condensed matter, has become an important experimental tool. A complete, *ab initio*, microscopic description of such a system comprising a positron embedded in an electronic medium has been recently given within the ECCM, using gauge-field techniques.

5. Summary

The CCM has proven itself to be an extremely versatile formulation of quantum many-body theory. At the practical level it is capable both of systematic improvement in principle through systematic hierarchies of approximations, and of achieving extremely high accuracy in practice at relatively low levels of implementation. At the purely formal level, recent developments, particularly with the extended (ECCM) version, have shown it also to be capable of embodying and describing many fundamental modern concepts of quantum many-body theory and quantum field theory. We expect that the method will continue to be developed and to grow even further in importance over the next decade, particularly for fundamental applications in quantum field theory.

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References

[1] F. Coester, *Nucl. Phys.* **7** (1958) 421.
[2] F. Coester and H. Kümmel, *Nucl. Phys.* **17** (1960) 477.
[3] H. Kümmel, *Theor. Chim. Acta* **80** (1991) 81.
[4] K.A. Brueckner, *Phys. Rev.* **100** (1955) 36.
[5] J. Goldstone, *Proc. Roy. Soc. (London)* **A239** (1957) 267.
[6] J. Hubbard, *Proc. Roy. Soc. (London)* **A240** (1957) 539.
[7] A. Hugenholtz, *Physica* **23** (1957) 481, 533.
[8] M. Gell-Mann and F. Low, *Phys. Rev.* **84** (1951) 350.
[9] A.L Fetter and J.D. Walecka, *Quantum Theory of Many-Particle Systems* (McGraw-Hill, New York, 1971).
[10] R.F. Bishop, *Theor. Chim. Acta* **80** (1991) 95.
[11] R.F. Bishop and H.G. Kümmel, *Phys. Today* **40-3** (1987) 52.
[12] R.F. Bishop and K.H. Lührmann, *Phys. Rev. B* **17** (1978) 3757.
[13] H. Kümmel, K.H. Lührmann and J.G. Zabolitzky, *Phys. Rep.* **36C** (1978) 1.
[14] V. Kvasnička, V. Laurinc and S. Biskupič, *Phys. Rep.* **90C** (1982) 160.
[15] J. Arponen, *Ann. Phys. (NY)* **151** (1983) 311.
[16] H. Kümmel, in *Nucleon-Nucleon Interaction and Nuclear Many-Body Problems*, eds. S.S. Wu and T.T.S. Kuo (World Scientific, Signapore, 1984), p.46.
[17] K. Szalewicz, J.G. Zabolitzky, B. Jeziorski and H.J. Monkhorst, *J. Chem. Phys.* **81** (1984) 2723.
[18] R.F. Bishop, in *Recent Progress in Many-Body Theories*, (Lecture Notes in Physics, Vol. **198**), eds. H. Kümmel and M.L. Ristig (Springer, Berlin, 1984), p.310.
[19] J.S. Arponen, R.F. Bishop and E. Pajanne, *Phys. Rev. A* **36** (1987) 2519.

[20] J.S. Arponen, R.F. Bishop and E. Pajanne, *Phys. Rev. A* **36** (1987) 2539.
[21] R.J. Bartlett, *J. Phys. Chem.* **93** (1989) 1697.
[22] J.S. Arponen and R.F. Bishop, *Phys. Rev. Lett.* **64** (1990) 111; *idem., Ann. Phys. (NY)* **207** (1991) 171; *idem., Theor. Chim. Acta* **80** (1991) 289.
[23] J.S. Arponen, *Theor. Chim. Acta* **80** (1991) 149.
[24] R.F. Bishop, J. Arponen and E. Pajanne, in *Aspects of Many-Body Effects in Molecules and Extended Systems*, (Lecture Notes in Chemistry, Vol. **50**), ed. D. Mukherjee (Springer, Berlin, 1989), p. 79; R.F. Bishop and J.S. Arponen, *Int. J. Quantum Chem.: Quantum Chem. Symp.* **24** (1990) 197.
[25] K. Emrich, *Nucl. Phys.* **A351** (1981) 379; 397; K. Emrich and J.G. Zabolitzky, *Nucl. Phys.*, **A351** (1981) 439.
[26] R.F. Bishop, M.C. Boscá and M.F. Flynn, *Phys. Lett.* **A132** (1988) 440; *idem., Phys. Rev.* **A40** (1989) 3484.
[27] R.F. Bishop, *Anales de Fisica* **A89** (1985) 9.
[28] R.F. Bishop, J.B. Parkinson and Yang Xian, *Phys. Rev. B* **43** (1991) 13782; **44** (1991) 9425.
[29] M. Altenbokum, K. Emrich, H. Kümmel and J.G. Zabolitzky, in *Condensed Matter Theories*, Vol. **2**, eds. P. Vashishta, R.K. Kalia and R.F. Bishop (Plenum, New York, 1987), p. 389.
[30] G. Sanyal, S.H. Mandal and D. Mukherjee, *Chem. Phys. Lett.* **192** (1992) 55.
[31] R. Offermann, W. Ey and H. Kümmel, *Nucl. Phys.* **A273** (1976) 349; R. Offermann, *Nucl. Phys.* **A273** (1976), 368; W. Ey, *Nucl. Phys.* **A296** (1978) 189.
[32] B. Brandow, *Rev. Mod. Phys.* **39** (1967) 771.
[33] I. Lindgren, *Int. J. Quantum Chem.: Quantum Chem. Symp.* **12** (1978) 33.
[34] L.L. Foldy, *Phys. Rev.* **124** (1961) 649; **125** (1962) 2208.
[35] R.F. Bishop and K.H. Lührmann, *Phys. Rev. B* **26** (1982) 5523; and unpublished.
[36] K.A. Brueckner, *Phys. Rev.* **156** (1967) 204.
[37] K. Emrich and J.G. Zabolitzky, *Phys. Rev. B* **30** (1984) 2049.
[38] J.G. Zabolitzky, *Phys. Rev. B* **22** (1980) 2353.
[39] D.M. Ceperley and B.J. Alder, *Phys. Rev. Lett.* **45** (1980) 566; S.H. Vosko, L. Wilk and M. Nusair, *Can. J. Phys.* **58** (1980) 1200.
[40] P. Vashishta and K.S. Singwi, *Phys. Rev.* **B6** (1972) 875; *E* 4883.
[41] H. Kümmel, *Phys. Rev. C* **27** (1983) 765; G. Hasberg and H. Kümmel, *Phys. Rev. C* **33** (1986) 1367.
[42] B. Day, *Phys. Rev. Lett.* **47** (1981) 226; B. Day and J.G. Zabolitzky, *Nucl. Phys.* **A366** (1981) 221.
[43] R.J. Bartlett, *Theor. Chim. Acta* **80** (1991) 71.
[44] J. Arponen, R.F. Bishop, E. Pajanne and N.I. Robinson, *Phys. Rev. A* **37** (1988) 1065.