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FROM INTERACTING NUCLEONS TO HAMILTONIAN LATTICE GAUGE THEORIES: A UNIFIED MANY-BODY TREATMENT*

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ABSTRACT

What has since become known as the coupled cluster method (CCM) was invented some 35 years ago to calculate ground-state energies of closed-shell atomic nuclei. The method has since been extended in many different ways to the point where it is nowadays recognized as providing one of the most universally applicable, most powerful, and numerically most accurate of all *ab initio* methods in the microscopic quantum many-body theory of finite or infinite systems. We review here the applications within nuclear physics, and thereby show how the CCM provides a unifying approach of almost unique stature. The early calculations on both closed- and open-shell nuclei and on infinite nuclear matter are thus related to the recent extensions which provide both extremely accurate calculations for light nuclei and a framework for handling various problems in nuclear field theory. The latter include pion-nucleon field theory and such Hamiltonian lattice gauge field theories as the Abelian $U(1)$ model and the non-Abelian $SU(2)$ model. In all cases we stress the underlying concepts and the high quality of the results obtained.

1. Introduction

When what has since become known as quantum hadrodynamics (QHD) was invented some 20 years ago by Walecka,¹ Willets and others,^{2,3} it was clear that a field-theoretical approach of this sort would be necessary for a description of matter at sufficiently high densities, such as those found in neutron stars. Nevertheless, it was still widely felt at that time that at the densities pertaining to stable terrestrial atomic nuclei, and for not too high excitation energy, the mesonic degrees of freedom could be eliminated in favour of static two-body internucleon potentials, with no observable loss. It was only some 15 or so years ago that sufficiently accurate many-body calculations were available for a range of closed-shell nuclei,⁴ for doubt to begin to be cast on this view (or hope). Although it took considerably longer for the majority of the nuclear physics community to become convinced, it is clear that the calculations done up to that time by Kümmel and his collaborators⁴⁻⁶ using the coupled cluster method (CCM) invented very much earlier by Coester and Kümmel⁷ for the express purpose of dealing with closed-shell nuclei, were very powerful. In particular, they were already sufficient to answer firmly in the negative the question posed by Bethe as to whether conventional static two-body potentials between

*This article is dedicated to João da Providência, friend and colleague, in honour of his 60th birthday.

nucleons are sufficient to describe the ground and low-lying energy levels of terrestrial nuclei to within experimental accuracy.

The CCM was the only method then available that satisfied the dual criteria of being both a true microscopic technique with a controlled hierarchy of approximations, and one which was demonstrably able to be implemented to sufficiently high levels in such a scheme to demonstrate convergence of the results to a much higher level of accuracy than the observed discrepancy with experiment, for a wide range of nucleon-nucleon forces. Later extensions of the CCM to deal with open-shell nuclei^{8,9} also showed comparable disagreement between experiment and fully converged calculations using two-body potentials.¹⁰ Similar calculations using CCM techniques were later performed by Day,¹¹ and show a similar inability to reproduce the 'experimental' saturation properties of infinite nuclear matter with two-body forces. All of these calculations demonstrated the need to include systematically *all* effects of three-body (and, to a certain extent, also the important four-body) correlations in the nuclear many-body system, in order to obtain converged results.

It is worth noting in the above regard that the latter CCM results of Day¹¹ were the culmination of the resolution of the so-called *crisis in nuclear matter theory* (and see, e.g., Ref. [12]) that occupied a central role in quantum many-body theory in the latter half of the 1970's. The fundamental issue was the observed disagreement between the lowest-order Brueckner theory (LOBT) calculations of the time-independent perturbation theory approach and various variational calculations, when both were performed with the same internucleon potential. By about 1975 many calculations showed that the expectation value of the Hamiltonian in a trial wavefunction of Jastrow form could be appreciably *lower* than the corresponding result from LOBT. The Rayleigh-Ritz variational principle then led inexorably to the conclusion that the Brueckner estimate had to be badly wrong, once one had accepted that the variational expectation value in the trial Jastrow state had been accurately evaluated by the available cluster-expansion techniques then employed. Day demonstrated explicitly¹³ that if the Brueckner-Bethe hole-line expansion approach is used to extend LOBT, then it is vital to include at least all three hole-line (Bethe-Faddeev) terms to obtain both convergence and agreement with the best variational estimates. Day then later showed¹¹ how such terms were most easily taken into account in a fully systematic fashion within the framework of the CCM.

The role played by the CCM in nuclear theory enacted at the level of nucleons interacting via static two-body forces is difficult to overestimate. In the past 10-15 years the method has also been applied to an increasingly diverse array of systems in condensed matter physics. An overview of these applications has been given recently by the present author.¹⁴ The method is nowadays widely perceived as providing one of the most powerful, most widely applicable, and numerically most accurate of all fundamental techniques of quantum many-body theory. The method itself has been adequately reviewed several times in recent years,¹⁴⁻²⁰ and we do not intend to do more here than sketch the underlying concepts in Sec. 2.

Instead, our main goal is to show that the CCM can provide an equally powerful

tool to describe nuclei and nuclear matter not only at the level of nucleons alone, but also at the quantum field-theoretical level where the relativistic propagation of the nucleons and the retarded propagators of the virtual meson fields are taken explicitly into account. Very recent work on applications to simple low-dimensional lattice gauge models [e.g., $U(1)$ and $SU(2)$] even holds out the exciting hope that the CCM might eventually be capable of handling the full complexity of the quantum chromodynamics (QCD) of the quarks and gluons that comprise the most fundamental constituents of the nucleon according to our present understanding.

Ultimately, nuclear theorists will need to explore the inter-relationships between these three different 'layers of physical reality' in nuclear physics. One (and perhaps the only) way to do this will be to use a unified microscopic quantum many-body/field theory approach which is capable, both in principle and in practice, of being applied to all the various models. We believe that the CCM is the only proven contender for such an assignment. Our aim in Secs. 3-5 is to review the evidence for this stance by surveying some of the relevant existing calculations.

2. Elements of the CCM

The exact ket and bra ground-state (g.s.) eigenvectors, $|\Psi_0\rangle$ and $\langle\tilde{\Psi}_0|$, of a many-body system described by a Hamiltonian H ,

$$H|\Psi_0\rangle = E_0|\Psi_0\rangle ; \quad \langle\tilde{\Psi}_0|H = E_0\langle\tilde{\Psi}_0| , \quad (1)$$

are parametrized within the CCM in the following fashion,

$$\begin{aligned} |\Psi_0\rangle &= e^S|\Phi\rangle ; \quad \langle\tilde{\Psi}_0| = \langle\Phi|\tilde{S}e^{-S} , \\ S &= \sum_I 's_I C_I^\dagger ; \quad \tilde{S} = 1 + \sum_I '\tilde{s}_I C_I . \end{aligned} \quad (2)$$

A basic ingredient is the model or reference state $|\Phi\rangle$, which plays the role of a vacuum state with respect to a suitable set of *mutually commuting* (many-body) multiconfigurational creation operators $\{C_I^\dagger\}$ and their hermitian conjugate destruction counterparts $\{C_I\}$,

$$C_I|\Phi\rangle = 0 , \quad I \neq 0 , \quad (3)$$

where $C_0 \equiv 1$, the identity operator. These operators are complete in the many-body Hilbert (or Fock) space $\mathcal{H}$,

$$1 = |\Phi\rangle\langle\Phi| + \sum_I 'C_I^\dagger|\Phi\rangle\langle\Phi|C_I , \quad (4)$$

where the prime on the sum over the configuration space label set $\{I\}$ (which denotes all possible multiparticle cluster configurations with respect to $|\Phi\rangle$) thus excludes the identity operator explicitly. Mathematically, the state $|\Phi\rangle$ plays the role of a cyclic vector, with respect to which the complete algebra in $\mathcal{H}$ is decomposed into two Abelian subalgebras.

We note that although the manifest hermiticity, $(\langle\tilde{\Psi}_0|)^{\dagger} = |\Psi_0\rangle$, is lost, the normalization condition $\langle\tilde{\Psi}_0|\Psi_0\rangle = \langle\Phi|\Psi_0\rangle = \langle\Phi|\Phi\rangle \equiv 1$, is explicitly imposed. The coefficients $\{s_I, \tilde{s}_I\}$ are regarded as being independent parameters, even though formally we have the relation,

$$\langle\Phi|\tilde{S} = \frac{\langle\Phi|e^{S^{\dagger}}e^S}{\langle\Phi|e^{S^{\dagger}}e^S|\Phi\rangle} . \quad (5)$$

They provide a complete description of the ground state. In particular, the g.s. expectation value of an arbitrary operator A is given as,

$$\bar{A} \equiv \langle\tilde{\Psi}_0|A|\Psi_0\rangle = \langle\Phi|\tilde{S}e^{-S}Ae^S|\Phi\rangle = \bar{A}[s_I, \tilde{s}_I] . \quad (6)$$

Furthermore, the coefficients $\{s_I, \tilde{s}_I\}$ may be determined variationally by requiring the g.s. energy expectation functional $\bar{H}[s_I, \tilde{s}_I]$ to be stationary with respect to all independent variations. We thus easily derive the coupled sets of equations,

$$\delta\bar{H}/\delta\tilde{s}_I = 0 \Rightarrow \langle\Phi|C_Ie^{-S}He^S|\Phi\rangle = 0, \quad I \neq 0, \quad (7)$$

$$\delta\bar{H}/\delta s_I = 0 \Rightarrow \langle\Phi|\tilde{S}e^{-S}[H, C_I^{\dagger}]e^S|\Phi\rangle = 0, \quad I \neq 0. \quad (8)$$

One may easily verify that Eqs. (7) and (8) are fully equivalent to the ket and bra g.s. Schrödinger equations (1). The linear set of equations (8) for $\tilde{S}$ may formally be solved as,

$$\langle\Phi|\tilde{S} = \langle\Phi| + \langle\Phi|e^{-S}He^SQ(E_0 - Qe^{-S}He^SQ)^{-1}Q, \quad (9)$$

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

$$Q \equiv 1 - |\Phi\rangle\langle\Phi|. \quad (10)$$

Equation (9) may be formally used to express an arbitrary g.s. expectation value $\bar{A} = \bar{A}[s_I, \tilde{s}_I]$ in Eq. (6) wholly in terms of the cluster coefficients $\{s_I\}$ alone. Furthermore, Eq. (7) easily shows that the g.s. energy E_0 at the stationary point is given by the particularly simple form,

$$E_0 = E_0[s_I] = \langle\Phi|e^{-S}He^S|\Phi\rangle \quad (11a)$$

$$= \langle\Phi|He^S|\Phi\rangle = \langle\Phi|H|\Psi_0\rangle. \quad (11b)$$

Very importantly, although this (bi-)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 preserved in all such approximate truncations.*

The set of equations (7) represents a coupled set of nonlinear equations for the c-number cluster coefficients $\{s_I\}$, in terms of the solution to which Eq. (11a) gives the g.s. energy, for example. Due to the nested commutator expansion,

$$e^{-S}He^S = H + [H, S] + \frac{1}{2!}[[H, S], S] + \cdots, \quad (12)$$

and the fact that all of the individual components of S in Eq. (2) commute with one another, each element of S in Eq. (2) is linked directly to the Hamiltonian in each of the terms of Eq. (12). Thus, each of the coupled equations (7) is of linked-cluster type. Furthermore, the otherwise infinite series of Eq. (12) always terminates here after a finite number of terms if, as is usually the case, each term in the second-quantized form of the Hamiltonian H contains a finite number of destruction operators, defined with respect to $|\Phi\rangle$. For a system of nucleons interacting via two-body forces, for example, Eq. (12) terminates after the term of fourth order in S . Equations (7) are therefore of finite order, and need no additional (artificial or approximate) truncation. This is in sharp contrast with the unitary-transformation equivalent of the underlying CCM similarity transformation 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 $|\Psi_0\rangle$.

In summary, the CCM explicitly preserves the important Goldstone linked-cluster theorem, and all g.s. expectation values given by Eq. (6) are linked-cluster quantities. Thus, both size-extensivity (which assures that the expectation values of extensive operators scale properly with particle number N) and the Hellmann-Feynman theorem are preserved at all levels of approximation. Such approximations within the CCM now simply amount to the restriction of the otherwise complete set of multi-configuration labels $\{I\}$ to some suitable finite or infinite subset, within some well-defined hierarchical scheme. We then solve the resulting Eqs. (7) and (8) *without making, and without the need to make, any further (what would usually be uncontrolled) approximations.*

Excited states $|\Psi_\lambda\rangle$ (or, more generally, states with zero overlap with $|\Phi\rangle$, as compared to the state(s) with nonzero overlap found by the g.s. formalism above) are now constructed in the CCM²¹ in terms of a set of linear excitation operators $\{X^\lambda\}$,

$$|\Psi_\lambda\rangle = X^\lambda|\Psi_0\rangle = X^\lambda e^S|\Phi\rangle; \quad X^\lambda = \sum_I x_I^\lambda C_I^\dagger. \quad (13)$$

Hence, the operators X^λ and S commute. The excited-state (e.s.) Schrödinger equation,

$$H|\Psi_\lambda\rangle = E_\lambda|\Psi_\lambda\rangle \equiv (E_0 + \epsilon_\lambda)|\Psi_\lambda\rangle, \quad (14)$$

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

$$e^{-S}[H, X^\lambda]e^S|\Phi\rangle = \epsilon_\lambda X^\lambda|\Phi\rangle, \quad (15a)$$

$$(e^{-S}He^S - E_0)X^\lambda|\Phi\rangle = \epsilon_\lambda X^\lambda|\Phi\rangle, \quad (15b)$$

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. (15a) or Eq. (15b) with each retained 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 $Q(e^{-S}He^S - E_0)Q$

as needs to be inverted to obtain $\tilde{S}$, as in Eq. (9). We also note that by taking the overlap of Eq. (15b) with $\langle\Phi|\tilde{S}$, we may easily prove, using Eqs. (7) and (11a), that the orthogonality condition $\langle\tilde{\Psi}_0|\Psi_\lambda\rangle = 0$ is preserved, provided $\epsilon_\lambda \neq 0$.

The above *single-reference version* of the CCM is most suited to so-called *closed-shell systems* for which a single choice of reference state $|\Phi\rangle$ provides a good starting point for the inclusion of correlations. In nuclear physics applications, for example, this would be the case for closed-shell nuclei, for which a single Slater determinant of occupied single-particle (s.p.) orbitals is a convenient choice for $|\Phi\rangle$. One can show that the formalism described may be written in such a way that when iterated one generates the non-degenerate version of time-independent perturbation theory (TIPT). In diagrammatic terms, one makes easy contact with the Goldstone diagrams of TIPT, and our basic Eqs. (7) and (11a) may be viewed as a direct embodiment of the Goldstone linked cluster theorem for the energy. For *open-shell systems* it is usually more appropriate to use a *multi-reference version* of the CCM^{8,9} which incorporates the linked-valence expansion of Brandow²² in the context of degenerate many-body TIPT, and its usual diagrammatic expression in terms of folded diagrams.

For pedagogical purposes, we describe the elements of this multi-reference CCM for the specific case of open-shell nuclei. Thus, we start with a neighbouring closed-shell system of N nucleons with exact g.s. energy $E_0 \rightarrow E_0^N$, and whose single-reference CCM model state is $|\Phi\rangle \rightarrow |\Phi_N\rangle = \prod_{i=1}^N a_{\mu_i}^\dagger |0\rangle$, the usual Slater determinant formed from the lowest N s.p. states of some complete s.p. set $\{|\alpha\rangle = a_\alpha^\dagger |0\rangle\}$, where $|0\rangle$ is the particle vacuum and the s.p. operators $\{a_\alpha^\dagger\}$ and their adjoints obey the usual fermionic commutation relations. We now add valence particles (or holes) one at a time. For the $(N+1)$ -particle system, the set of Slater determinants $\{a_i^\dagger |\Phi_N\rangle; i \in \mathcal{V}\}$, where $\mathcal{V}$ is some set of degenerate or quasi-degenerate valence orbitals, are viewed as a set of reference states which should be kept together for the low lying states $\{\Gamma\}$ that we wish to construct. We may thus distinguish three sorts of s.p. orbitals $\{\alpha\}$, namely: (i) orbitals occupied in $|\Phi_N\rangle$ (labelled $\alpha \rightarrow \mu, \nu, \dots$); (ii) valence orbitals (labelled $\alpha \rightarrow i, j, \dots \in \mathcal{V}$) partially occupied by the valence particles outside the core; and (iii) the remaining "unoccupied" orbitals (labelled $\alpha \rightarrow \rho, \sigma, \dots$). We now wish as far as possible to incorporate the *exact* solution of the N -body closed-shell core, and to add explicitly the extra correlations arising from the valence particles. In this way we are led to the following multi-reference CCM ansatz for the exact $(N+1)$ -particle states,

$$|\Psi_{N+1}^\Gamma\rangle = \sum_{i \in \mathcal{V}} e^S [1 + F^{(1)}] a_i^\dagger |\Phi_N\rangle \kappa_i^\Gamma. \quad (16)$$

The c-number coefficients $\{\kappa_i^\Gamma\}$ in Eq. (16) determine the particular admixture of Slater determinants in the model state, and the operator $F^{(1)} = \sum_{n=1}^{N+1} F_n^{(1)}$ describes the dressing of the bare valence particle by its interactions with the core. Its one-body partition, $F_1^{(1)}$, for example, describes the one-body (Hartree-Fock) part of the valence problem, whereas $F_2^{(1)}$ describes the *core polarization* terms which arise from the correlations between the valence particle and any one core particle, etc. These operators are easily written explicitly in second-quantized form.

The comparable two valence-particle $(N+2)$ -body wavefunction ansatz is,

$$|\Psi_{N+2}^A\rangle = \sum_{i,j \in \nu} e^S \left[1 + F^{(1)} + \frac{1}{2} : F^{(1)^2} : + F^{(2)} \right] a_i^\dagger a_j^\dagger |\Phi_N\rangle \kappa_{i,j}^A, \quad (17)$$

where the factor of $\frac{1}{2}$ 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 $F^{(2)} = \sum_{n=2}^{N+2} F_n^{(2)}$. If we proceed to add more valence particles outside the core in a similar fashion, we rapidly arrive at the normal-ordered exponential ansatz first written down by Lindgren,²³ although the formulation of Ey⁹ is wholly equivalent.

By inserting Eqs. (16) and (17) into the respective $(N+1)$ - and $(N+2)$ -body Schrödinger equations, and premultiplying by the usual factor e^{-S} , one is readily led to equations for the energy eigenvalues E_T^{N+1} and E_Δ^{N+2} . Suitable projections onto the model space lead to secular equations for the admixture coefficients κ_i^Γ and κ_{ij}^A . It can be shown^{8,17} 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 many-body TIPT), with eigenvalues equal to the respective excitation energies (e.g., $\epsilon_\Gamma \equiv E_T^{N+1} - E_0^N$). Similar projections out of the model space onto "unoccupied" states lead to equations which determine the matrix elements of the operators $F^{(1)}$ and $F^{(2)}$. The interested reader is referred to the literature already cited for further details of these and the by now many other extensions of the CCM.

3. The Nucleus as Nucleons Interacting via Static Potentials

Many applications of the CCM have been made for finite nuclei interacting via a range of static two-body potentials, both with and without the inclusion of additional static three-body potentials.^{4,10,17,21,24-26} These studies have been for both such closed-shell nuclei as ^4He , ^{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 reached from them by the addition of one or two valence particles or holes. Most calculations have been for the g.s. energy and the excitation spectrum. We note here that the theory of the effective interaction has been very fully investigated with the multi-reference CCM,^{8,9} so that the spectrum of an open-shell nucleus may be calculated either completely microscopically, by using only the Hamiltonian as input, or semi-microscopically, by also using experimental information on the single-particle excitation energies $\{\epsilon_\Gamma\}$. The relationships between the e.s. version of the single-reference CCM and the earlier multi-reference CCM have also been explored in detail,²¹ via the theory of the effective interaction. In this way the excited states of closed-shell nuclei have also been calculated semi-microscopically by making use of experimental s.p. energies, as well as fully microscopically. Calculations have also been made for the momentum distribution²⁴ and the density distribution^{4,17}

of the nucleons inside a nucleus, and for the elastic electron-scattering form factor.²⁶ In the latter case, the effects of the explicit inclusion of exchange currents due to π, ω and ρ mesons were also taken into account, in a very early calculation of this type.

It is probably fair to say that by contrast with most previous calculations, and even with some still being done, especially in the case of open-shell nuclei, essentially all of the CCM calculations on both finite nuclei and nuclear matter are demonstrably converged. For that reason it has been possible to draw the conclusions discussed in Sec. 1 concerning the inadequacy of local two-body (and probably even two-body plus three-body) forces for describing accurately even the low-lying energy levels of atomic nuclei and the saturation properties of nuclear matter.

Since the above conclusions are by now relatively well known, we content ourselves here with not showing again the detailed results which provide the evidence on which they rest. The interested reader may easily discover them in the literature cited. Rather, we wish to stress some of the technical details of the calculations and the approximations involved. One of the most important concerns the truncation systematics. An obvious partitioning of S into n -body pieces, $S = \sum_{n=1}^N S_n$, where S_n creates n particle-hole (ph) pairs from the Slater determinant model state, $|\Phi\rangle \rightarrow |\Phi_N\rangle$, leads to the so-called SUB n scheme in which all partitions S_m with $m > n$ are set to zero. The hard-core (or strongly repulsive) nature of the internucleon interaction at short distances, however, precludes the implementation of such a scheme, which is ill-defined in the extreme hard-core limit. Similar problems arise within TIPT where finite-order Goldstone diagrams are also ill-defined. As is well known, the solution for this problem within TIPT is to re-express the perturbation series by replacing the bare potential V by its dressed Brueckner-Bethe-Goldstone G -matrix counterpart. Each bare interaction is thereby replaced by an infinite ladder sum.

This basic idea of grouping interaction lines V into ladder series can also be incorporated within the CCM. Indeed, such diagrammatic structures are generated automatically at even the very low SUB2 level of approximation. However, even the SUB2 approximation generates many more terms than just the ladder diagrams.¹⁵ Where problems arise in the SUB n scheme with hard-core potentials is that the replacement of a bare potential *everywhere* in the Goldstone diagrams so generated by the iteration of the truncated CCM equations, leads also to diagrams which are not included at the same n th-order level.

However, the cure is simple. Thus, in a given SUB n approximation one first identifies that maximal subset of terms which when retained and iterated lead only to diagrams which are still contained in this same class when each bare interaction V is replaced by a ladder sum or G -matrix, and when the relative time-ordering of the remaining interactions is kept fixed. The resulting (hard-core) truncation scheme is called the HCSUB n scheme, and it is closely related to the hole-line expansion of Bethe.^{4,16,17} The CCM calculations on the closed-shell nuclei^{4,17,21,24,25} and on nuclear matter¹¹ have all been performed up to the HCSUB4 level, with the two- and three-body terms in the resulting equations treated exactly, and at least the most important

contributions of the rather complicated four-body terms also retained. The retention of all such terms is vital for convergence to accurate results. The calculations on open-shell nuclei^{10,17} were performed to a similar order in a comparable truncation scheme involving also the operators $F^{(n)}$.

We also note that, in principle, any truncated CCM calculation will depend on the choice of s.p. basis $\{|\alpha\rangle = a_\alpha^\dagger|0\rangle\}$ used to construct the Slater determinant reference states. This sensitivity to the choice of s.p. basis at a given HCSUBn level of truncation can, indeed, be used as an internal check on the convergence. Several choices of s.p. basis have been proposed and used, which, *a priori*, are difficult to choose between on theoretical grounds.^{4,14} It is, therefore, gratifying to find that for all nuclei studied, the results are indeed rather insensitive to any reasonable choice of basis.

A final technical point concerns the general fact that model reference states $|\Phi\rangle$ often violate some exact symmetry. An important example here is that unless the s.p. orbitals are plane waves (as for the case of infinite homogeneous nuclear matter), the state $|\Phi\rangle$ is not an eigenstate of the total momentum operator $\mathbf{P}$, and hence not translationally invariant. Although the exact states should be simultaneous eigenstates of H and $\mathbf{P}$, the exact translational invariance is generally not preserved in SUBn or HCSUBn approximations. Most calculations on nuclei have dealt with this problem by using the internal Hamiltonian,

$$H \rightarrow H_{\text{int}} \equiv H - T_{\text{CM}} \quad , \quad (18)$$

where $T_{\text{CM}} = \mathbf{P}^2/2M$ is the kinetic energy operator of the centre of mass (CM), and M is the total mass. For N nucleons of mass m each and momenta $\{\mathbf{p}_i\}$, interacting via pairwise potentials V_{ij} , the internal Hamiltonian is

$$H_{\text{int}} = \left(1 - \frac{1}{N}\right) \sum_{i=1}^N \frac{\mathbf{p}_i^2}{2m} + \sum_{i < j=1}^N \left(V_{ij} - \frac{\mathbf{p}_i \cdot \mathbf{p}_j}{Nm}\right) \quad . \quad (19)$$

The main effect of the removal of the CM energy is thus to produce a momentum-dependent interaction. All of the calculations reported above have been performed using the H_{int} of Eq. (19). Undoubtedly, at any level of approximation its use is a compromise between the exact Eq. (11a) and the fact that the exact g.s. is an eigenstate of $\mathbf{P}$, and neglecting the CM motion entirely.

Fortunately, this approximation has been checked for the ${}^4\text{He}$ nucleus in a recent series of papers,²⁷⁻²⁹ using a translationally invariant cluster method (TICM), which is a variant of the CCM specially invented to incorporate translational (and rotational) invariance *exactly* at all levels of approximation. One finds that the error incurred by the use of H_{int} in the standard CCM described is no worse than the errors involved in the neglect of higher-order terms, at any level of truncation. On the other hand, the TICM has completely eliminated the problem of spurious CM motion which has so bedevilled calculations on finite nuclei. Although the TICM has originally been cast in a form which makes for easy comparison with standard generalized shell-model

approaches,²⁷ it may also much more conveniently and powerfully be expressed wholly in a coordinate-space basis.^{28,29} Finally, this work²⁹ also shows particularly clearly the increasing insensitivity to the s.p. basis as the order of the approximation is increased, in a very accurate calculation for the ⁴He nucleus using a model state $|\Phi\rangle$ comprised of 0s harmonic oscillator orbitals with a variable oscillator frequency.

4. The Nucleus via Meson-Nucleon Field Theory

Most successful parametrizations of the nucleon-nucleon potential, including some of those used in the calculations discussed in Sec. 3, have incorporated at least one-boson exchange (OBE), particularly for the long-range part. It is therefore clear, even at this level, that the dynamical presence of mesons should also be taken into account explicitly within the nuclear medium. We are thus led to consider field-theoretical Hamiltonians which underlie the OBE potentials. We consider in this Section two such models to which the CCM has been applied.

4.1. The Lee Model and Nuclear Matter

The Lee model³⁰ contains three kinds of particles V , N and θ , with the only allowed transition being $V \rightleftharpoons N + \theta$, and which may be loosely identified with the neutron, proton and negative-pion respectively. In a second-quantized notation in which the respective fermion creation operators are $V_\alpha^\dagger$ and $N_\beta^\dagger$, and the θ -boson creation operator is $b_k^\dagger$ (where α, β and k specify completely the s.p. states), the Lee model is defined by the Hamiltonian,

$$\begin{aligned} H &= H^0 + W + W^\dagger, \\ H^0 &= \sum_\alpha E_\alpha^0 V_\alpha^\dagger V_\alpha + \sum_\beta E_\beta N_\beta^\dagger N_\beta + \sum_k \omega_k b_k^\dagger b_k, \\ W &= \sum_{\alpha, \beta, k} W_{\alpha\beta k}^0 V_\alpha^\dagger N_\beta b_k. \end{aligned} \quad (20)$$

The Lee model is a particularly simple field theory in that the one- and two-body problems can be solved explicitly. Thus, the renormalization effects are especially simple due to the lack of antiparticles and since H commutes with both the "baryon number" operator $B \equiv \sum_\alpha V_\alpha^\dagger V_\alpha + \sum_\beta N_\beta^\dagger N_\beta$, and the "charge" operator $Q \equiv \sum_\beta N_\beta^\dagger N_\beta - \sum_k b_k^\dagger b_k$. In particular, the trivial states $|\beta\rangle \equiv N_\beta^\dagger|0\rangle$ and $|k\rangle \equiv b_k^\dagger|0\rangle$, where $|0\rangle$ is the vacuum, are the exact "proton" and "pion(π^-)" eigenstates with $(B, Q) = (1, 1)$ and $(0, -1)$ respectively. The corresponding s.p. energies thus remain unrenormalized, and are given as $E_\beta \equiv (p_\beta^2 + M^2)^{\frac{1}{2}}$ and $\omega_k \equiv (k^2 + \mu^2)^{\frac{1}{2}}$ in terms of "physical" masses M and μ respectively. By contrast, the physical "neutron" state is an admixture of the bare "neutron" state $V_\alpha^\dagger|0\rangle$ and the "proton-pion" states $|\beta k\rangle \equiv N_\beta^\dagger b_k^\dagger|0\rangle$ which co-exist in the $(B, Q) = (1, 0)$ sector. One can easily

show that the unrenormalized quantity E_α^0 in Eq. (20) may be eliminated in favour of a "physical" or renormalized quantity $E_\alpha \equiv (p_\alpha^2 + M^2)^{\frac{1}{2}}$. In a similar fashion, the bare vertex function $W_{\alpha\beta k}^0$ is renormalized to a "physical" dressed value $W_{\alpha\beta k}$ which depends only on $W_{\alpha\beta k}^0$, E_α , E_β and ω_k .

The Lee model of symmetric nuclear matter (i.e., equal numbers of neutrons and protons) is now defined by the sector $(B, Q) = (2N, N)$ for $N \rightarrow \infty$. An obvious model state is a direct product of the bosonic vacuum with the usual fermionic filled Fermi sea, $|\Phi\rangle \rightarrow |\Phi_F\rangle = \prod_{a,b \in \mathcal{F}} V_a^\dagger N_b^\dagger |0\rangle$, where $\mathcal{F}$ denotes the set of N lowest plane-wave states up to some Fermi momentum p_F . The correlation operator S in Eq. (2) now takes the schematic form

$$S = S_{aBk}^{101} N_B^\dagger V_a b_k^\dagger + S_{abAB}^{110} N_B^\dagger V_A^\dagger V_a N_b + S_{aa'AA'}^{200} V_{A'}^\dagger V_A V_a V_{a'} \\ + S_{bb'BB'}^{020} N_{B'}^\dagger N_B^\dagger N_b N_{b'} + S_{abBB'k}^{111} N_{B'}^\dagger N_B^\dagger V_a N_b b_k^\dagger + \dots, \quad (21)$$

in a hopefully self-evident notation with summation convention implied, and where the labels (a, b) denote occupied and (A, B) denote unoccupied s.p. (V, N) states respectively, with respect to $|\Phi_F\rangle$. In general, the operator $S = \sum_{k,l,m} S^{klm}$, where the operator S^{klm} creates k V -holes, l N -holes and m θ -mesons from $|\Phi_F\rangle$. By the symmetries of the Lee Hamiltonian the general term in S^{klm} contains all possible linear combinations of products containing $(k-m)$ $V_A^\dagger$ -operators, $(l+m)$ $N_B^\dagger$ -operators, k V_a -operators, l N_b -operators and m $b_k^\dagger$ -operators, all of which commute between themselves.

We note that Bodden³¹ has performed a numerical CCM calculation for this Lee model of nuclear matter in an approximation which retains only the partitions S^{101} and S^{110} (so that, crudely speaking, the important effects of N - θ and N - V scattering are included). The renormalization of the masses and vertices in the one-particle (V) case is replaced in the infinite matter problem by the renormalization of energy denominators and correlation functions in his calculations. It is very gratifying to find that even this relatively crude approximation leads to stable N - V model nuclear matter, albeit at too low a saturation density and too low an energy per particle compared with the "physical" values for real nuclear matter, when the free parameters in the Lee model are fitted to the corresponding parameters for real nucleons and pions. This is perhaps to be expected, however, primarily since the real world also contains π^+ and π^0 mesons. Less importantly, some possibly significant effects have been neglected from the calculation. For example, although V - V and N - N scattering can only occur through the exchange of at least two θ -particles in this model, one ought to investigate the effect of including also the partitions S^{200} and S^{020} which would generate them.

It is also interesting to note that a unitary form of the e^S ansatz, namely where $|\Psi_0\rangle$ is parametrized as in Eq. (2) but $\langle\tilde{\Psi}_0|$ is taken as its manifest hermitian conjugate was advocated for use in field theory by da Providência and Shakin³² over 20 years ago. This variational method leads to an *infinite* expansion for E_0 even when S is truncated, and hence suffers from the drawbacks mentioned in Sec. 2 by comparison

with the CCM. Nevertheless, it has also been formally applied³³ to the Lee model of nuclear matter discussed here, although no numerical results were reported.

4.2. Pseudoscalar Pion-Nucleon Field Theory and the Deuteron

A rather different and more realistic application of the CCM described in Sec. 2 is provided by the standard (3+1)-dimensional model of pions and nucleons interacting via an isospin-invariant pseudoscalar coupling. The model is described in terms of the Hamiltonian $H = \int d^3x \mathcal{H}(\mathbf{x})$ with density

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

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

$$\mathcal{H}_{\text{int}} = \mathcal{H}_{\text{int}}(\mathbf{x}) = -ig \int d^3x' F(\mathbf{x} - \mathbf{x}') \bar{\Psi}_{t'}(\mathbf{x}) \gamma_5 \tau_t \Psi_{t'}(\mathbf{x}) \Phi_t(\mathbf{x}') , \quad (22)$$

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 $\bar{\Psi}_{t'}(\mathbf{x})$ are respectively the (fermionic) four-component Dirac nucleon field operator and its adjoint. The matrices $\boldsymbol{\gamma}$ 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

$$F(\mathbf{q}) = \frac{\lambda^2 - m_0^2}{\lambda^2 + q^2} , \quad (23)$$

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 performed³⁴ within the multi-reference ("open-shell") formulation described in Sec. 2. The *physical* vacuum $|\Psi_0\rangle$ is first written in terms of the *bare* vacuum as model state, $|\Phi\rangle \rightarrow |0\rangle$, as in Eq. (2). The cluster correlation operator S is now expanded as a double sum, in terms of the number m of pions and the number n of nucleon-antinucleon pairs virtually excited, $S = \sum_{m,n} S_{mn}$, with $m + n > 0$. Secondly, the (physical) one-nucleon state is treated exactly as in the one-valence parametrization of Eq. (16); and, thirdly, the two-nucleon state is treated as in the two-valence parametrization of Eq. (17). The operators $F^{(1)}$ and $F^{(2)}$ are also decomposed as for S above into (m, n) partitions.

Such a multi-reference CCM calculation has been performed by Hasberg and Kümmel,³⁴ in which they retained the partitions $S_{01}, S_{11}, F_{10}^{(1)}$ (and $F_{20}^{(1)}, F_{01}^{(1)}$ and $F_{11}^{(1)}$ 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 experimental pion mass of 139 MeV. The one-nucleon calculation was then used to fit the bare mass M_0 so as to give an 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 calculated. 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, corresponding bare nucleon masses of $M_0 = 726, 664$, and 651 MeV 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 pleasing 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 to achieve the corresponding physical value and with a value for $g^2/4\pi$ reduced by only a factor of 1.28 from the above physical value.

The above calculations clearly go *far* beyond the inclusion of OBE effects, in a completely non-perturbative way. All indications are that these very impressive pioneering calculations are close to full convergence, since even in the truncation used only relatively few terms contribute strongly, and all terms of higher order seemed to be numerically small.

5. Hamiltonian Lattice Gauge Theories

One of the founders of lattice QCD, namely Wilson, claimed some four years ago³⁵ that before the subject can meaningfully interact with experiment we need *both* an increase in computing power of at least 10^8 *and* a comparable increase in the power of the algorithms. His suggested solution was to try methods from quantum chemistry. In view of the fact that the CCM is now one of the methods of first choice in this field,¹⁹ where state-of-the-art CCM calculations are now done for molecules with up to 80 or more active electrons, we decided about two years ago to explore the usefulness of the CCM for lattice gauge field theory (LGFT), and we report briefly here on some of our progress to date.³⁶⁻³⁹

We note that Wilson's comments above were made in the context that the most common way of solving LGFT models was, and still is, to sample the global Lagrangian action using the Metropolis algorithm in a typical Monte Carlo calculation. Nevertheless, one may also treat the Hamiltonian form of LGFT as a many-body problem. For example, in the simple Abelian case of $U(1)$, corresponding to quantum electrodynamics (QED), the group element on a link ℓ originating at a lattice site with position vector $\mathbf{n}$ in (positive) direction $\mathbf{k}$ may be written as $U_{\mathbf{k}}(\mathbf{n}) = \exp[iA_{\mathbf{k}}(\mathbf{n})]$, and the corresponding Hamiltonian as

$$H = \frac{1}{2} \sum_{\mathbf{k}, \mathbf{n}} E_{\mathbf{k}}^2(\mathbf{n}) + \lambda \sum_{\mathbf{k}, \mathbf{n}} [1 - \cos B_{\mathbf{k}}(\mathbf{n})] , \quad (24)$$

where $E_k(\mathbf{n})$ is the electric field on the links and $B_k(\mathbf{n})$ is the magnetic field defined as the lattice curl,

$$B_i(\mathbf{n}) = \epsilon_{ijk}[A_k(\mathbf{n} + \mathbf{e}_j) - A_k(\mathbf{n})] , \quad (25)$$

around the elementary plaquettes defined by the unit lattice vectors $\mathbf{e}_i$. Conventional electrodynamics is recovered when the lattice spacing shrinks to zero and only the $\frac{1}{2}B^2$ term remains from the expansion of the cosine. Quantum mechanics is imposed in the temporal gauge via the fundamental commutation relation, $[A_k(\mathbf{n}), E_{k'}(\mathbf{n}')] = i\delta_{kk'}\delta_{\mathbf{n}\mathbf{n}'}$, which may be realized by the representation $E_k(\mathbf{n}) \rightarrow -i\partial/\partial A_k(\mathbf{n})$. Using this representation and Eq. (25) it is not difficult to write H wholly in terms of plaquette variables, in the gauge-invariant sector. In (1+1) or (2+1) dimensions, for example, we find in a self-evident plaquette notation,

$$H = \sum_p \left[-2 \frac{\partial^2}{\partial B_p^2} + \lambda(1 - \cos B_p) \right] + \sum_{\langle p, p' \rangle} \frac{\partial^2}{\partial B_p \partial B_{p'}} , \quad (26)$$

where the second sum over $\langle p, p' \rangle$ indicates all nearest-neighbour pairs of plaquettes. As a by-product of treating space as a discrete lattice in order to cure the ultraviolet divergence problems, $U(1)$ LGFT is thus reduced to an infinite many-body problem with compact variables, $-\pi < B_p \leq \pi$.

In the non-Abelian $SU(N)$ case the basic variables are the $SU(N)$ matrices defined on each link ℓ in terms of the $N^2 - 1$ group generators, and the conjugate "chromo-electric" fields E_ℓ^a have $N^2 - 1$ components. For example, in the case of $SU(2)$, the group element on each link has the general form $U = d_0 \mathbf{1} + i \sum_{i=1}^3 d_i \sigma_i$, where the σ_i are the usual Pauli matrices, and the real coefficients d_α satisfy $\sum_{\alpha=0}^3 d_\alpha^2 = 1$, and hence lie on a sphere in four-dimensional Euclidean space. The potential term in Eq. (24) generalizes to $\lambda \sum_p [N - \text{Re Tr } U_p]$, where $U_p = U_1 U_2 U_3 U_4$ for the plaquette formed from the four links $l = 1, 2, 3, 4$ in cyclic order. Further details may be found in the literature.⁴⁰

Our primary aim is now to parametrize the physical (gauge-invariant) ground and excited ("glueball") states of the above Hamiltonian in the vacuum sector (i.e., the charge-free sector for $U(1)$ or the "quark-free" sector for $SU(N)$, particularly $N = 3$), by CCM forms exactly as in Sec. 2. Our first need is thus to choose a suitable model state $|\Phi\rangle$. For ease of discussion let us henceforth focus on the $U(1)$ model of Eq. (26) in (1+1) or (2+1) dimensions. A convenient choice is the so-called electric (or strong-coupling, $\lambda \rightarrow 0$) vacuum $|0\rangle$, for which $E_\ell|0\rangle = 0$ for all ℓ . Equivalently, the one-plaquette Hamiltonian obtained from Eq. (26) reduces in the $\lambda \rightarrow 0$ limit to $H_0 = -2d^2/dB^2$ with the two sets of eigenstates $\{\cos mB; m = 0, 1, 2, \dots\}$ with even parity and $\{\sin mB; m = 1, 2, \dots\}$ with odd parity. The corresponding g.s. is clearly a constant. We thus take $|\Phi\rangle \rightarrow C$, a c -number. We may now define the n -plaquette correlation operators S_n , with $S = \sum_{n=1}^{N_p} S_n$, where $N_p \rightarrow \infty$ is the number of plaquettes on the lattice as

$$S_1 = \sum_{n=1}^{\infty} \sum_{p=1}^{N_p} S_p(n) \cos nB_p , \quad (27a)$$

$$S_2 = \frac{1}{2!} \sum_{n_1, n_2=1}^{\infty} \sum_{p_1, p_2=1}^{N_p} ' \left[S_{p_1 p_2}^{(1)}(n_1, n_2) \cos n_1 B_{p_1} \cos n_2 B_{p_2} + S_{p_1 p_2}^{(2)}(n_1, n_2) \sin n_1 B_{p_1} \sin n_2 B_{p_2} \right], \quad (27b)$$

etc., where the prime on the sum in Eq. (27b) excludes the term with $p_1 = p_2$. In this way the whole CCM machinery can be put into effect, with excited states, for example, treated in an analogous fashion via the general Eq. (13).

Practically, we may implement either the standard SUB n truncation scheme as discussed previously or a new *local* truncation scheme, called LSUB n , where we neglect both all correlations between m plaquettes with $m > n$ and all correlations between $m < n$ plaquettes if those m plaquettes occupy a region on the lattice which cannot be delimited by at most n contiguous plaquettes. Further sub-truncations in both schemes can be performed in terms of the numbers $\{n_k\}$ of modes kept in the sums in Eq. (27). These mode numbers $\{n_k\}$ bear a direct relationship with the winding numbers of the equivalent Wilson loops retained in the CCM approximation for S . Indeed, in this latter context, it should be clear how to generalize our approach to $SU(N)$ LGFT, at least in principle.

We have also performed³⁹ some preliminary calculations using an alternative *mean-field-like* model state $|\Phi\rangle \rightarrow |\Phi_{mf}\rangle = e^T|0\rangle$, where $T = \frac{1}{2}t \sum_{p=1}^{N_p} \cos B_p$, and the parameter t is optimised in some suitable fashion. Details of the results of all such calculations can be found elsewhere.³⁶⁻³⁹ We remark only that these preliminary investigations of the Abelian $U(1)$ LGFT are very encouraging. We have seen how specific truncations exactly reproduce strong-coupling perturbation theory (PT) in the $\lambda \rightarrow 0$ limit. They comprise, in effect, a well-defined analytic continuation or resummation of such PT series, within the context of a natural and consistent hierarchy, and are *far* superior to the usual *ad hoc* approaches based on generalized Padé approximants. We find g.s. energies and glueball masses in good agreement with previous accurate results, even for $\lambda \sim 10$, which is *far* into the weak-coupling regime. Preliminary work on the non-Abelian $SU(2)$ model³⁹ has also been carried out at the SUB1 level, where we reproduce earlier results of Robson and Webber.⁴¹ More detailed results for this model, including correlation effects, have also been obtained recently⁴² by a technique which uses the same basic (exponential) parametrization of the wavefunctions as our Eqs. (2) and (13), but which does not use the standard form of the CCM.

6. Summary

In the very limited space available we have attempted to demonstrate that the elements of the CCM both provide us with a many-body formalism of immensely wide applicability, and one which is also capable of yielding results of very high accuracy in practice. When applied to the standard model of finite nuclei and infinite nuclear matter as collections of nucleons interacting via static potentials, the *fully*

converged results disagree with experiment at much lower energies than might have been expected beforehand for a model without mesons. It is interesting to note that the added input of just a few data from experiment (viz., the s.p. energy levels), does improve the situation considerably, however. Indeed, the CCM can be formulated in such a way as to provide a rigorous basis for many of the standard concepts of nuclear theory, such as collective motion or the shell model with effective interactions, which also rely on some fitting parameters which, ideally, should be calculated microscopically.

We have seen too how the same basic CCM technology which was originally invented for the above purposes, has also very successfully been applied to field-theoretical models of nucleons and mesons. Very recent further extensions to lattice gauge theory lead us to hope that it might not be unrealistic to expect that the CCM may also give results that help to bridge the enormous gap that still exists between present-day calculations in QCD and experiment.

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