BRUECKNER THEORY WITH JASTROW WAVE FUNCTIONS

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ABSTRACT

A unification of Brueckner and Jastrow ideas is pursued with the aim of combining the advantages of the hole-line-expansion and variational approaches, while avoiding their disadvantages. The unified theory is achieved by adapting the coupled-cluster or exp(S) formalism to a basis of Jastrow-correlated wave functions. On the one hand, this formulation permits the systematic inclusion of non-Jastrow (particularly, state-dependent) correlations into the description of the ground state. On the other hand, the Jastrow correlations serve to tame the bare interaction to the extent that simple truncations of the new system of coupled-cluster equations may yield reliable results for interesting many-body problems involving realistic interactions and realistic densities. For the case of nuclear matter, a "correlated Bethe-Goldstone equation" is proposed which in effect sums the generalized ladder diagrams of correlated-basis perturbation theory.

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1. INTRODUCTION

The subtitle "Jastrow Correlations versus Brueckner Theory" chosen for the third topical school sounds controversial. This is in keeping with the circumstance that in the past there has been little progress in establishing practical methodological connections between the two major approaches to solution of the ground-state many-body problem.

By contrast, the title of our contribution seems to promise something like a "grand unification". This comparison is certainly exaggerated considering the present state of development and application of the theory we shall propose. Nevertheless, we shall be able to demonstrate that the Brueckner-Jastrow controversy is, in the larger view, quite artificial, and that "Brueckner theory" can be applied without any conceptual or practical difficulties in situations where a good share of the two-body correlation effects are already described by Jastrow-correlated wave functions. In fact, the "correlated Brueckner theory" to be proposed below will emerge as just an important special case of a much more general many-body theory built on a basis of correlated wave functions. Another important special case will involve summation of correlated RPA ring diagrams.

Before taking up the necessary formali ٦, which will be adapted here to the infinite Fermi medium, let us discuss in a ـit more detail the motivation for improvising a combined Jastrow-Brueckner theory and the ideas which underlie our realization of this objective. Procedures have been developed in the past five years [1-3] which make possible the accurate calculation of the expectation value of the Hamiltonian with respect to a Jastrow trial state

$$|\Psi_0> = F|\Phi_0> , \quad F = \prod_{1\le i<j\le A} f(r_{ij}) \quad . \tag{1}$$

The model ket $|\Phi_0>$ is supposed here to be the ground state of the corresponding system of noninteracting particles--a Slater determinant of plane waves filling a Fermi sea. The procedures we have in mind are generally referred to as Fermi hypernetted-chain (FHNC) methods and are available in several versions (e.g., the Krotscheck-Ristig version [1,4], the Fantoni-Rosati version[2] and a hybrid called FHNC/C [5]). Some aspects of these methods are discussed in the accompanying lectures of Rosati [6]. The computational effort required for the calculation of the energy expectation value

$$E_{var}[f] = <\Psi_0|H|\Psi_0>/<\Psi_0|\Psi_0> \tag{2}$$

in any of the FHNC procedures as normally practiced is very modest (less than one second CPU time on a Cyber 76) for a typical Jastrow trial function around the nuclear-matter saturation density. If we choose to determine f(r) by the variational prescription

$$(\delta E_{var}[f]/\delta f)(r) = 0 \tag{3}$$

as considered in refs. [7,4,8-9], the price we pay is an increase in computer time by

a factor of order ten (based on an efficient program). However, in return we obviate the often cumbersome search for a suitable parameterized choice of f(r), and, moreover, we may obtain as a bonus a single-quasiparticle excitation spectrum and quasiparticle interaction simply by a few algebraic manipulations.

To give an explicit account of the construction of the quasiparticle energies and interaction is a non-trivial task beyond the scope of this contribution. Though these quantities are in fact the basic ingredients of our "correlated Brueckner theory", it will suffice for the coming presentation to know that, in the special case of a Jastrow correlation operator (1), they can be determined without much effort beyond that already needed for the energy expection value (2). One may refer to the original literature [10,8-9] for details; an outline of the essential structural results is provided in accompanying lecture notes [11].

Look now at the simple, state-independent Jastrow ansatz (1) for the wave function. Clearly, it has deficiencies which cause it to be only a moderately accurate or even a poor description of nature: It does not reflect the complexity of realistic nuclear interactions (spin and isospin dependence, presence of tensor and spin-orbit components, etc.), nor does it include the effects of "backflow" or spin-density fluctuations, which are apparently quite significant in liquid ^{3}He. The most obvious way to improve upon this situation is to replace the Jastrow function $f(r_{ij})$ by a (two-body) Jastrow operator, f(ij), and replace the product (1) by the symmetrized product of the f(ij). Fermi-hypernetted-chain-type theories predicated on special forms of state-dependent correlation operators F have been studied [12-16]; progress in this direction is discussed to some extent in the lectures of Rosati [6] (see also ref. [17]). Such theories are, however, still in a state of flux; considerably more work is needed before a convincing, definitive version can emerge. In any event these approaches, with the exception of a few simple cases [15-16], inevitably sacrifice much of the elegance and transparency of state-independent FHNC theory.

Difficulties of this kind are not present in Brueckner theory. An arbitrarily complicated two-body interaction conforming to the required symmetry principles can be readily accomodated, since it enters the theory quite conveniently in terms of its partial wave expansion. The problems with Brueckner theory center instead on questions about its convergence. In particular, if the Brueckner-Bethe hole-line approach is adopted it is necessary to execute at least the three-hole-line, Bethe-Faddeev summation for a quantitative estimate of the saturation properties of nuclear matter to be obtained [18]. More generally, the simultaneous summation of ladder and ring diagrams requires, in the case of strong interactions, the inclusion of Bethe-Faddeev terms [19]. In liquid ^{3}He, even these elaborations would seem to be insufficient to account for the experimental ground-state energy and density at equilibrium. We point out in addition that a Brueckner (more properly, Brueckner-Bethe) calculation at the three-hole-line level is extremely laborious, demanding some hours of CPU time on a very large computer.

Thus we conclude that the advantages and disadvantages of "Jastrow" and "Brueckner" theories are in fact almost complementary, the former being characterized by good convergence and complicated descriptions of state dependence, the latter by questionable convergence and unproblematic description of state dependence.

It is therefore natural to try to join the two approaches (meaning in particular state-independent Jastrow theory and "lowest-order" Brueckner theory) in such a way as to combine their advantages while eliminating their disadvantages. This leads us to the idea of "Brueckner theory with Jastrow wave functions". The plan of action is simple:

(i) Use a Jastrow correlation operator to describe in an approximate (or, in a sense, average) way the short-range dynamical correlations in the system. Of course, the long-range correlations emerging from the solution of the variational problem (3) may also be built in.

(ii) Construct a weak (or at least weakened) "residual" or "effective" interaction, which will be responsible for introducing all those effects which are not taken care of by the Jastrow ansatz.

(iii) Improve upon the description of the many-body system by perturbation theory. As a special example one might sum all particle-ladder diagrams defined in terms of the effective interaction, by means of a "correlated Bethe-Goldstone equation".

This idea is not new; in fact it is implicit in the method of correlated basis functions (CBF) [19-21]. However, practical applications of this idea have remained limited to the calculation of second-order perturbation corrections. In step (iii) above one envisions a systematic analysis of non-orthogonal CBF perturbation theory paralleling the Goldstone analysis of the familiar Rayleigh-Schrödinger perturbation expansion. The aim of course is to identify certain topologically defined classes of terms (e.g., ring and ladder diagrams or self-energy corrections) and to sum them by integral equation techniques. A straightforward implementation of this program has been obstructed by some rather uncomfortable technical complications [22] which we will touch upon later. Progress toward the stated goal was made only recently through the development of the so-called "correlated coupled-cluster theory" (CCC) [23]. A "correlated Bethe-Goldstone equation" arises naturally as the keystone of a special case of this theory.

The ideas and assumptions of our unification of Brueckner and Jastrow approaches will be further delineated in the next two sections. In section 2 we shall review the elements of the CBF scheme and sketch the coupled-cluster procedure of Coester and Kümmel [19]. The latter provides a very efficient means for generating Bethe-Goldstone-like theories with correlated wave functions. A diagrammatic representation convenient for pursuing CCC theory is introduced in section 3. Space does not allow the inclusion of complete derivations (which at any rate are more technical

than instructive). Rather, we shall confine ourselves to a description of the essential building-blocks and to an outline of the essential steps. For the details the reader must consult the original publication [23].

We conclude in section 4 with a discussion of systematic approximation procedures within the new theory, and with some remarks on the physical problems to be attacked in the near future. Our path will lead us finally back to state-dependent variational theories, which maintain an appeal to those who prefer to think in terms of correlation functions. Thus, by a judicial averaging technique applied to the CCC equations, we shall see how a state-dependent "variational" treatment corresponding to a desired correlation-operator structure can be generated to order. One may obtain in this manner not only the appropriate energy expression, but also equations for the state-dependent correlation components analogous to the optimization condition (2).

2. CORRELATED COUPLED-CLUSTER THEORY

The principles of correlated-basis-functions theory [19-21] have already been covered in lectures at this school by one of us [11]. Accordingly, we can herein restrict ourselves simply to defining the quantities which will be needed in the forthcoming treatment of the infinitely extended Fermi system. The correlation operator F is employed to produce a set of normalized, but nonorthogonal, correlated wave functions or state vectors

$$|\psi_m\rangle = F|\Phi_m\rangle I_{mm}^{-\frac{1}{2}} \quad , \qquad I_{mm} \equiv \langle\Phi_m|F^\dagger F|\Phi_m\rangle \quad , \tag{4}$$

from a complete orthonormal set of Slater determinants $|\Phi_m\rangle$. The label $m = \{m_1 \ldots m_A\}$ specifies the plane-wave orbitals entering $|\Phi_m\rangle$, i.e.,

$$|\Phi_m\rangle = (A!)^{-\frac{1}{2}} \, |m_1 \ldots m_A\rangle_a \quad , \tag{5}$$

where the subscript $\underline{a}$ means "antisymmetrized". The special label o is reserved for the completely filled Fermi sea (cf. (1)). In the correlated basis $\{|\psi_m\rangle\}$ we define:

(i) Diagonal matrix elements of the Hamiltonian,

$$H_{mm} = \langle\psi_m|H|\psi_m\rangle \quad , \tag{6}$$

as well as differences thereof which will be identified with differences of single-particle energies e. For an n particle-n hole (np-nh) state $|\Phi_m\rangle = a_{p_1}^\dagger \ldots a_{p_n}^\dagger \, a_{h_1} \ldots a_{h_n} |\Phi_o\rangle$ one can write [10]

$$H_{mm} - H_{oo} = \sum_{i=1}^{n} \left(e_{p_i} - e_{h_i}\right) + O(A^{-1}) \quad .$$

(We shall adhere to the convention [11] of denoting particle orbitals by p_i and hole orbitals by h_i.)

(ii) Off-diagonal matrix elements of the unit operator and the Hamiltonian,

$$N_{mn} = \langle\psi_m|\psi_n\rangle \ , \qquad H_{mn} = \langle\psi_m|H|\psi_n\rangle \qquad (m \neq n) \tag{8}$$

with

$$J_{mn} = N_{mn}(1 - \delta_{mn}) \ . \tag{9}$$

The non-diagonal H elements need appear only in the combination [11]

$$H'_{mn} = (H_{mn} - H_{oo}N_{mn})(1 - \delta_{mn}) \ . \tag{10}$$

It is also convenient to introduce the combination [10-11]

$$W_{mn} = H_{mn} - \frac{1}{2}(H_{mm} + H_{nn})N_{mn} \ . \tag{11}$$

A perturbation series for the ground-state energy, analogous to that of Rayleigh-Schrödinger theory, can now be formulated [21] in terms of the quantities (6)-(10). Displaying terms through fourth order, this expansion reads

$$E = H_{oo} - \sum_m \frac{H'_{om}H'_{mo}}{H_{mm} - H_{oo}} + \sum_{mn} \frac{H'_{om}H'_{mn}H'_{no}}{(H_{mm} - H_{oo})(H_{nn} - H_{oo})} +$$

$$+ \left[- \sum_{mnp} \frac{H'_{om}H'_{mn}H'_{np}H'_{po}}{(H_{mm} - H_{oo})(H_{nn} - H_{oo})(H_{pp} - H_{oo})} + \sum_{mn} \frac{H'_{om}H'_{mo}H'_{on}H'_{no}}{(H_{mm} - H_{oo})^2(H_{nn} - H_{oo})} \right.$$

$$\left. - \sum_{mn} \frac{J_{om}H'_{mo}H'_{on}H'_{no}}{(H_{mm} - H_{oo})(H_{nn} - H_{oo})} - \sum_{mn} \frac{H'_{om}J_{mo}H'_{on}H'_{no}}{(H_{mm} - H_{oo})(H_{nn} - H_{oo})} \right] + \ldots \ . \tag{12}$$

As an initial step in the application of the CBF perturbation series (12) we have to specify the sets of states to be included in the summations which appear. An obvious characterization is by means of the number d of orbitals in which the various model states differ from each other, and from the filled Fermi sea. By virtue of translational invariance, d = 2 is the simplest non-trivial case for the uniform, infinite medium. Given two model states $|\Phi_m\rangle$, $|\Phi_n\rangle$ differing in d orbitals, with say $|\Phi_m\rangle = a^\dagger_{m_1} \ldots a^\dagger_{m_d} a_{n_d} \ldots a_{n_1} |\Phi_n\rangle$, we may define non-local d-body operators $N(1\ldots d)$ and $W(1\ldots d)$ which recapture the CBF quantities N_{mn} and W_{mn}, respectively, through

$$N_{mn} = J_{mn} = \langle m_1 \ldots m_d | N(1\ldots d) | n_1 \ldots n_d \rangle_a \equiv N_{m_1\ldots m_d, n_1\ldots n_d} \ , \tag{13}$$

$$W_{mn} = \langle m_1 \ldots m_d | W(1\ldots d) | n_1 \ldots n_d \rangle_a \equiv W_{m_1\ldots m_d, n_1\ldots n_d} \ . \tag{14}$$

Although not so indicated explicitly, the operators $N(1\ldots d)$ and $W(1\ldots d)$ also depend, in detail, on the underlying state $|\Phi_n\rangle$; however, this dependence does not enter the

theory on the level at which we choose to present it here, with the exception that $N(1\ldots d)$ and $W(1\ldots d)$ fail to be Galilean invariant. For completeness we mention also that the diagonal limit of the off-diagonal matrix elements of the effective two-body interaction $W(12)$, denoted $\langle ij|W(12)|ij\rangle_a$, may be related to Landau's quasi-particle interaction.

It is in principle possible to crank out perturbation corrections of arbitrary order and analyze the resulting expansion by stepwise, pedestrian application of the basic CBF machinery set up for example in refs. [20,21]. Very soon, however, one is faced with manipulative tasks of formidable scale [22], not least due to the occurrence of unlinked nonorthogonality corrections, which cancel in different orders of the perturbation series. For example, there are unlinked $d = 4$ contributions in the second-order term of the expansion (12) which cancel against unlinked $d = 2$ contributions to the fourth-order term (see the last two addends given explicitly in (12)). Thus, if we are confined to this straightforward treatment, unphysical contributions with catastrophic dependence on the particle number must be tediously rooted out and eliminated by hand. Ideally, we would like to find a more efficient machinery which automatically generates the physical contributions wholesale--without the necessity for overt cancellation of unlinked addends. (This might be partially accomplished, for example, through iteration of a suitable integral equation resembling the Bethe-Goldstone equation. In order to find a mechanism of the desired sort, we must go back to conventional, "uncorrelated" many-body theories and look for a comprehensive non-perturbative formalism suitable for generalization to the CBF context.

Having stated the problem in these terms, the coupled-cluster (or exp(S)) approach of Coester and Kümmel [19] suggests itself as a most expedient remedy to our formal troubles. In the conventional form of coupled-cluster theory, the exact ground state is expressed as

$$|\chi_o\rangle = e^S|\Phi_o\rangle \tag{15}$$

where

$$S = \sum_{n=2}^{A} S^{(n)} \quad , \tag{16}$$

$S^{(n)}$ being a superposition of operators which produce out of the Fermi-sea "vacuum" an n-particle, n-hole configuration. The $S^{(n)}$ are determined by the Schrödinger equation, written in the form

$$\langle\Phi_m|e^{-S}\,H\,e^{S}|\Phi_o\rangle = E\,\delta_{mo} \quad , \tag{17}$$

for all np-nh states $|\Phi_m\rangle$. The suitability of truncated versions of the representation (16) of S and the set of equations (17) will depend on the nature of the physical system under consideration. If we wish to extract, for special approximations, the Bethe-Goldstone equation or (for weak forces) the RPA equation, it will suffice to retain only $S^{(2)}$. This is not the place to pursue further details of the

coupled-cluster formalism. An appreciation of its generality and elegance may be gained from the recent review by Kümmel, Lührmann and Zabolitzky [19].

Returning to the central idea of CBF theory, we may explicitly incorporate any prescribed correlations into the coupled-cluster framework, by application of a suitable correlation operator F (e.g., the state-independent Jastrow choice). This operator is applied not simply to the Fermi sea as in ordinary variational theory, but rather to a superposition of Slater determinants, represented in the exp(S) manner. Thus we express the exact ground state as

$$|\chi_0\rangle = F e^S |\Phi_0\rangle \ . \tag{18}$$

Just as in the conventional exp(S) theory, we determine S through the Schrödinger equation, written now in the form

$$e^{-S} F^\dagger H F e^S |\Phi_0\rangle = E e^{-S} F^\dagger F e^S |\Phi_0\rangle \ . \tag{19}$$

Eliminating the ground-state energy E via

$$E = \langle\Phi_0|e^{-S} F^\dagger H F e^S |\Phi_0\rangle / \langle\Phi_0|e^{-S} F^\dagger F e^S |\Phi_0\rangle \tag{20}$$

and projecting (19) on a set of np-nh states $|\Phi_m\rangle$, we arrive after appropriate normalization at the set of "correlated coupled-cluster" (CCC) equations

$$\frac{\langle\Phi_m|e^{-S} F^\dagger H F e^S |\Phi_0\rangle}{\langle\Phi_0|e^{-S} F^\dagger F e^S|\Phi_0\rangle} = \frac{\langle\Phi_0|e^{-S} F^\dagger H F e^S |\Phi_0\rangle\langle\Phi_m|e^{-S} F^\dagger F e^S|\Phi_0\rangle}{\langle\Phi_0|e^{-S} F^\dagger F e^S|\Phi_0\rangle^2} \ . \tag{21}$$

It is now time to specify the first choice of approximations which serve to convert the exact yet intractable set of equations (20)-(21) into a solvable problem. In concert with our aim of deriving a generalized edition of the Bethe-Goldstone equation, we shall agree to retain only the 2p-2h term $S^{(2)}$ of S. Consistent with this approximation, we shall keep only those off-diagonal matrix elements of $F^\dagger HF$ and $F^\dagger F$ (or portions of such off-diagonal elements) which can be expressed purely in terms of one of the non-local two-body operators $W(12)$ and $N(12)$ or of unlinked products of these operators. (Note that this does <u>not</u> imply specialization to d = 2, since, for example, $W(1234)$ contains unlinked components of the type $W(12)N(34)$, etc. We keep all contributions having such a product structure.) These two restrictions, which amount to a species of "independent-pair" approximation (cf. ref. [14]), may later be relaxed without formal difficulty to permit the inclusion of Bethe-Faddeev contributions and/or effective three-body interaction and nonorthogonality operators produced by the Jastrow factor. We shall refrain from this elaboration not only for clarity, but also because practical applications will of course first concentrate on the simplest case.

Before turning, in the next section, to the more technical part of this paper, namely the derivation of the explicit equations for the two-body "amplitude" $S^{(2)}$,

we should emphasize that our theory is not limited to the state-independent Jastrow choice (1) for the correlation operator. Other, state-dependent, forms may be employed as well, but of course that would call for an appropriate extension of the existing formalism [10] for the construction of the non-local two-body operators $W(12)$ and $N(12)$.

3. TWO-PARTICLE AMPLITUDES

Our task now is the formulation of more explicit equations for the 2p-2h amplitude contained in

$$S = S^{(2)} = \frac{1}{(2!)^2} \sum_{p_1 p_2 h_1 h_2} S_{p_1 p_2 (h_1 h_2)_a} \, a^\dagger_{p_1} \, a^\dagger_{p_2} \, a_{h_2} \, a_{h_1} \tag{22}$$

and for the corresponding energy expression. Whereas in conventional coupled-cluster theory one can invoke the fact that the Lie series

$$e^{-S} H e^{S} = H + [H,S] + \frac{1}{2!} [[H,S],S] + \ldots \tag{23}$$

breaks off after the fourth-order commutator [19], we must deal with infinite cluster expansions of both the ground-state energy and the CCC equations. One possible scheme for generating such expansions is the "power-series" method [11]. To pursue this method we define a one-parameter energy function $E(\eta)$ by replacing S with ηS everywhere in the energy expression (20), and expand $E(\eta)$ in powers of η about $\eta = 0$. Note that we do not at this stage carry out cluster expansions in the correlations introduced by F; we simply assume that some algorithm exists for accurate calculation of all the required diagonal and off-diagonal CBF quantities (6)-(11). For the present, neither a commitment to a certain approximation for these quantities nor even a definite choice of the correlation operator F is necessary.

Writing out the resulting energy expression to leading non-trivial order (i.e., retaining the correction to the variational energy H_{oo} which is linear in S), we have

$$\begin{aligned} E &= H_{oo} + \langle \Phi_o | F^\dagger (H - H_{oo}) F S | \Phi_o \rangle \, I_{oo}^{-1} + O(S^2) \\ &= H_{oo} + \sum_m H'_{om} (I_{mm}/I_{oo})^{\frac{1}{2}} \, S_{mo} + O(S^2) \quad , \end{aligned} \tag{24}$$

where the sum in the last line runs over all labels m corresponding to 2p-2h states. Further analysis, involving terms of higher order in S, is, as usual, accelerated by a graphical notation. We adapt the Goldstone-like conventions of ordinary coupled-cluster theory:

(i) Particles (holes) are represented by solid lines with upward-(downward-) going arrows.

(ii) The 2p-2h operator yielding $(I_{mm}/I_{oo})^{\frac{1}{2}} S_{mo}$ is depicted by an ellipse.

(iii) The effective interaction $V(12)$ generating H'_{om} is symbolized by a horizontal wavy line. In the energy expansion, we need only the 2p-2h effective-interaction matrix elements. These may be written [10] quite simply in terms of the two-body versions of the operators N and W of (13)-(14) and the single-particle energies (7),

$$H'_{om} \equiv \langle h_1 h_2 | V(12) | p_1 p_2 \rangle_a$$
$$= \langle h_1 h_2 | W(12) | p_1 p_2 \rangle_a + \frac{1}{2} \left[e_{p_1} + e_{p_2} - e_{h_1} - e_{h_2} \right] \langle h_1 h_2 | N(12) | p_1 p_2 \rangle_a \quad . \tag{25}$$

More generally, the effective interaction operator $V(12)$ may be defined by

$$V_{\alpha\beta,\gamma\delta} \equiv \langle \alpha\beta | V(12) | \gamma\delta \rangle_a = W_{\alpha\beta,\gamma\delta} + \frac{1}{2} \left[\pm e_\alpha \pm e_\beta \pm e_\gamma \pm e_\delta \right] N_{\alpha\beta,\gamma\delta} \tag{26}$$

wherein the plus sign applies for particle states and the minus for hole states.

(iv) A single-particle (single-hole) energy, entering as a factor, will be represented by a dot on a particle (hole) line.

(v) The two-body normalization correction operator $N(12)$ is symbolized by a horizontal dashed line.

The calculation of higher-order corrections to the ground-state energy is rather tedious, though essentially straightforward. We by-pass the details and summarize the basic procedure to be followed:

(i) Expand the energy expression (20) in powers of $S^{(2)}$, noting that S operators appear only between F and $|\Phi_o\rangle$.

(ii) Insert a complete set of plane-wave Slater determinants between F and the S powers. For an nth-order term, only the 2np-2nh states give non-zero contributions.

(iii) Analyze the remaining off-diagonal matrix elements of $F^\dagger HF$ and $F^\dagger F$ according to their structure. Retain only the products describing independent pairs. Cancel unlinked diagrams. (It is in fact a non-trivial statement that the energy expansion is linked. This has to be proved for our construction.)

After performing the manipulations (i)-(iii) just listed, we may synthesize the following highly compact structural result:

The correction to the ground-state energy arising from the effective two-body interaction $V(12)$ may be expressed in the form

$$\Delta E = \frac{1}{4} \sum_{p_1 p_2 h_1 h_2} \langle h_1 h_2 | V(12) | p_1 p_2 \rangle_a \langle p_1 p_2 | \$^{(2)} | h_1 h_2 \rangle_a \quad , \tag{27}$$

where $\$^{(2)}$ is a 2p-2h operator (in the same sense as $S^{(2)}$) which can be formed entirely in terms of $S^{(2)}$ and the nonorthogonality correction operator $N(12)$. More precisely, the "renormalized" operator $\$^{(2)}$ may be represented graphically as the sum of all connected 2p-2h diagrams composed of arbitrary numbers of $S^{(2)}$ (ellipse)

elements and $N(12)$ (dashed line) elements with the provisos that

(i) No two N elements may be connected directly by a particle or a hole line and

(ii) All external lines enter S elements.

Some typical diagrams contributing to $\$^{(2)}$, featuring ring and ladder diagrams and a diagram with a factorizable insertion, are shown in fig. 1. It should be remarked that the structural result (27) is even more general than indicated in the above. The definition of $\$^{(2)}$ can be extended to allow for the incorporation of 3,4,...-particle S operators and normalization-correction operators, provided only that they are linked ultimately to a two-body operator. In this manner the partial resummation of the energy expansion represented by (27) can be made even more sweeping.

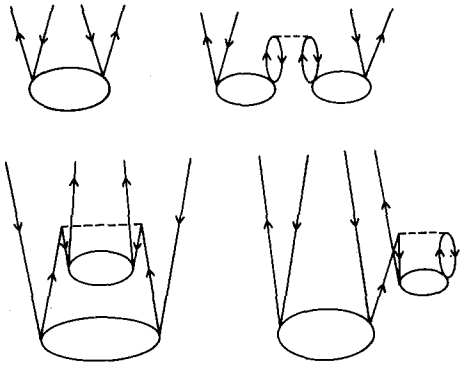

Figure 1
Typical diagrams contributing to $\$^{(2)}$.

Rather than presenting further calculation details, let us try to make the structural decomposition (27) plausible in elementary terms. First, it is clear that the energy expression must be linear in V; this just reflects the linearity of (20) in H. Second, there cannot be connections between any two N elements or between N and V elements. This is due to the fact that we have restricted ourselves to independent two-body operators. Third, all matrix elements of $F^{\dagger}HF$ (and consequently of $V(12)$) are to be taken between the ground model state $\langle\Phi_0|$ and some 2p-2h excited model state $|\Phi_m\rangle$. This is attributable to the fact that $\langle\Phi_0|e^{-S} = \langle\Phi_0|$.

Apart from the existence of induced effective 3, 4, ...n, ...-body interactions we have arrived at an energy expression which has precisely the same form as in conventional coupled-cluster theory. The distinctive feature of our treatment relative to the conventional one is that the role of the strong bare two-body interaction is taken over by a weak (or at least weakened) effective interaction. The latter is non-local and strictly multi-body in character, although the two-body

portion entering the result (27) is presumably dominant.

Of course, in spite of the formal beauty of expression (27), this result is of little use if we are forced to construct the renormalized 2p-2h operator $\$^{(2)}$ diagram by diagram from $S^{(2)}$ and N elements. To devise a more efficient approach which exploits the resummation implicit in (27), we have first to subject the correlated coupled-cluster equations (21) to the same process as we applied to the energy. That is, we have to expand (21) in powers of $S^{(2)}$ and analyze the resulting series diagrammatically. Since we aim only at deriving an equation for $S^{(2)}$, we restrict the bra vectors $\langle\Phi_m|$ to 2p-2h states. The calculational procedure exactly parallels that outlined above for E. Hence we will again by-pass the details and give only the final result.

The coupled-cluster equation (21) for $S^{(2)}$ is represented graphically by the statement that the sum of all 2p-2h diagrams of a certain class is zero. The diagrams of this class are characterized as follows:

(i) Two hole lines enter and two particle lines exit at the top of each such diagram; otherwise there are no external lines.

(ii) An arbitrary number of S and N elements may be present.

(iii) Precisely one effective-interaction operator V or one single-particle or hole energy e appears.

(iv) The S elements have only incoming hole lines and outgoing particle lines attached.

(v) No e, N or V element may be connected directly to a V element.

Sample diagrams of the above class are drawn in fig. 2. In the first two rows of the figure we see only diagrams already known from conventional exp(S) theory. The third row features additional corrections originating from the nonorthogonality of the correlated basis functions. Further graphs may, for example, be generated by exchange of two particle or two hole lines in the usual fashion of Goldstone diagrammatics, or by reversing the direction of a path described by particle and hole lines.

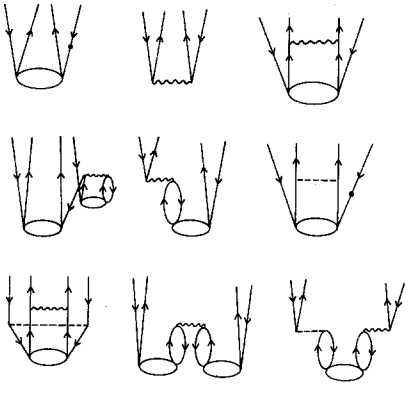

Figure 2
Typical diagrams entering the correlated coupled-cluster equations for $S^{(2)}$.

On proceeding with the cluster expansion of (21) there is a proliferation of more and more complicated diagrams containing additional S ellipses and normalization lines. Most significantly, we repeatedly encounter the same topological substructures as occur in the summation of S and *N* elements into the renormalized 2p-2h operator $. For example, corresponding to any of the "typical" diagrams of fig. 2 we are able to identify in the full expansion a series of diagrams in which, each in its turn, these substructures take the place of any of the S elements of the chosen typical diagram. Quite generally, we may in fact eliminate the original S operator entirely from the theory by replacing it with $\$^{(2)}$ wherever it appears, while imposing the additional restriction on the graphical representation of the CCC equations that:

(vi) No 2p-2h subdiagrams occur in which all external lines enter an $ operator, with the trivial exception of the diagram in which the only operator involved is the single $ operator.

By a 2p-2h subdiagram of a graph occurring in cluster expansion of the CCC equations, we mean a portion of the graph which can be separated off by cutting two particle lines and two hole lines.

We have, at this point, achieved a complete renormalization of the correlated coupled-cluster theory at the two-body level. With the elimination of $S^{(2)}$ in favor of $\$^{(2)}$, all infinite series of ladder and ring diagrams have been absorbed, along with other graphical subsets. The only graphical objects which remain on the surface are the renormalized diagrams which serve as "generators" of these infinite subsets (producing the ladders, rings, etc. upon iteration). Borrowing a term from variational theory, we may call these generator diagrams "elementary".

The formal part of our work has reached its goal, namely the derivation of general prescriptions for the calculation of the energy and the 2p-2h "amplitude" $S^{(2)}$ (or, more economically, $\$^{(2)}$) occurring in the correlated coupled-cluster theory. In the next section we may proceed with the discussion of truncation schemes expected to be useful in practical applications of our equations.

4. SUMMARY AND OUTLOOK

In this contribution we have shown that Brueckner and Jastrow approaches need not be in conflict. Far from being mutually exclusive, the two approaches may in fact be joined harmoniously within a unified theory (the CCC scheme) of great generality. Appropriating the correlated-basis functions idea, we may formulate "Brueckner theory" in a basis of correlated ("Jastrow") wave functions as easily as in a basis of independent-particle model functions. Although the first practical applications of the new, combined theory are still in progress, the standards of quality are predetermined. Since we combine the advantages of both of the older approaches and can, at the same time, avoid their disadvantages, we are bound to obtain a theory superior to both.

Let us see how to extract special cases from the general correlated coupled-cluster equations. The simplest measure is just to keep the driving term of the equations (i.e., the first two diagrams in fig. 2); then

$$\langle p_1 p_2 | \$^{(2)} | h_1 h_2 \rangle_a = - \left[e_{p_1} + e_{p_2} - e_{h_1} - e_{h_2} \right]^{-1} \langle p_1 p_2 | V(12) | h_1 h_2 \rangle_a \quad . \tag{28}$$

This leads us to the second-order CBF correction for the energy [21]. As a next step, we may retain additionally the particle-ladder diagrams, e.g., the third and sixth graphs of figure 2. The resulting equation is a sort of "correlated Bethe-Goldstone" equation:

$$\$^{BG}_{p_1 p_2 (h_1 h_2)_a} = - \left[e_{p_1} + e_{p_2} - e_{h_1} - e_{h_2} \right]^{-1} \left\{ V_{p_1 p_2 (h_1 h_2)_a} + \frac{1}{2} \sum_{pp'} \left[V_{p_1 p_2 (pp')_a} - \left(e_{h_1} + e_{h_2} \right) N_{p_1 p_2 (pp')_a} \right] \$^{BG}_{pp'(h_1 h_2)_a} \right\} \quad . \tag{29}$$

In equation (29), we still have the unmodified CBF single-particle (single-hole) energies. "Self-consistent" single-particle (or -hole) energies E may be introduced by inclusion of factorizable particle-line (or hole-line) insertions; thus

$$E_p = e_p - \frac{1}{2} \sum_{p'hh'} \$_{pp'(hh')_a} V_{hh'(pp')_a} \quad ,$$

$$E_h = e_h + \frac{1}{2} \sum_{h'pp'} V_{hh'(pp')_a} \$_{pp'(hh')_a} \quad . \tag{30}$$

As an alternative (or additional) step, we may include the "correlated RPA rings" by summing diagrams in the CCC equations typified by the fifth, eighth and ninth entries in fig. 2.

The type of equation to be solved finally will depend on the many-body system under consideration, the physical question we are asking and also on the correlation operator, i.e., the type of correlations which are incorporated explicitly via F. If the nuclear-matter problem is pursued with a state-independent F, solution of the correlated Bethe-Goldstone equation is surely the first thing to consider when implementing realistic nuclear interactions. The situation is rather different in liquid ^{3}He, where the short-range correlations may already be reasonably-well described by the Jastrow F. The most immediate problem in this system is the treatment of backflow correlations and spin-density fluctuations--otherwise, explanation of the effective mass, magnetic susceptibility and type of superfluid phase will be out of reach. (Parenthetically: one can show that the dominant part of the CBF effective interaction is associated with backflow correlations (see refs. [8,9]).) In liquid ^{3}He, it may in fact be more important to sum the generalized ring diagrams than the correlated ladder diagrams.

The same is true in the electron gas (one-component plasma). In this case definite information on the importance of non-Jastrow correlations is available. Calculation of the second-order energy correction in CBF perturbation theory applied to the electron gas [24] yields a result which at high densities (i.e., in the weak-

coupling regime) is in good agreement with the difference between Green-function Monte Carlo and variational Monte Carlo energies. On the other hand, in the low-density (strong-coupling) regime the predicted $\ln r_s$ behavior is not obtained with just the second-order correction, pointing to the necessity of including the generalized ring diagrams.

Finally, let us discuss the relation of our approach to purely variational methods, in which successive improvements upon the description of the ground-state wave function are made by introducing more and more elaborate correlation operators [12-17]. Both theories (CCC and purely variational) require the bare two-particle interaction to be represented in an operator basis rather than in a partial-wave decomposition. (Here, "operator basis" is meant in the sense of refs. [13,17].) In the purely variational theories one must, however, introduce a new correlation-operator component for each new component of the interaction, (re-)derive a suitable cluster expansion for the energy expectation value and determine somehow the detailed form of the new correlation ingredient. None of these steps is called for in the CCC theory. We need only know the action of each component of the interaction on the correlation operator F entering (18). For ease of discussion, we may take this to be a Jastrow factor. It turns out that all components of a v_{14} interaction [13, 17] act trivially on the Jastrow factor except the $\underset{\sim}{L}^2$ terms, which also do not engender any serious difficulty. Moreover, no extra prescription is needed to fix the detailed form of the non-Jastrow correlations; they are already determined by the CCC equations.

Another point of comparison concerns the technical complications associated with the derivation and summation of cluster expansions for state-dependent correlation operators. In the variational theories these complications manifest themselves in three classes of terms:

(i) Commutator contributions. Such contributions arise from the fact that in general two correlation operators referring to overlapping subsets of particles do not commute. The problem of disposing of commutator corrections does not occur in CCC theory, since all S operators and all terms of S operators commute by virtue of their p-h structure.

(ii) Chain diagrams. In contrast to cluster-expanded variational theory, infinite series of chain diagrams do not appear in the renormalized CCC scheme. Rather, their counterparts (the so-called RPA diagrams) are absorbed into a finite number of terms in an integral equation.

(iii) Parallel-connected diagrams. Similarly, parallel-connected or composite diagrams (more properly, their counterparts) are collected and removed from sight upon summation of the ladder diagrams of the original CCC equations.

It is very interesting to note that, in fact, the CCC approach may be used to manufacture equivalents of state-dependent variational theories, while circumventing

the problems indicated in (i)-(iii) above. This is done by averaging the CCC equations over the hole states, and approximating the average of a product of S, N and W ingredients by the product of their average values. To be more specific, we may (in a transparent notation) set up an averaging procedure

$$\langle S\rangle(q) = \sum_{hh'} S_{h+q,h'-q;hh'} \Big/ \left[\sum_{h} \Theta(k_F - |h|)\Theta(|h+q| - k_F)\right]^2 ,$$

$$\langle S^{\sigma}\rangle(q) = \sum_{hh'} S_{h+q,h'-q;hh'}\, g_1 \cdot g_2 \Big/ \left[\sum_{h} \Theta(k_F - |h|)\Theta(|h+q| - k_F)\right]^2 ,$$

$$\text{etc.}, \tag{31}$$

leaving the momentum transfer as the only independent variable, and perform the same operations on the equations. As a result of the stated process all the particle and hole lines of the CCC equations will reduce to combinations of the familiar exchange lines of diagrammatic Jastrow theory [3]. A potential advantage of this scheme is that we have to deal only with functions of one variable, thus facilitating the inclusion of more diagrams in the equations determining S.

At the present time it is not clear which way of treating the CCC equations is the most promising, i.e., whether it is more important to treat the state dependence of the correlations very accurately (as in the Bethe-Goldstone equation), paying for this the price of being able to include only a limited class of diagrams with reasonable effort, or if on the other hand one should include more diagrams in an "averaged" way. The decision will surely depend on the particular many-body system being attacked.

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