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ON BRUECKNER-BETHE AND COUPLED-CLUSTER MANY- BODY METHODS

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ABSTRACT

Partially summed perturbation series constitute one possible starting point for construction of theories of infinite and finite Fermion matter. I discuss various problems encountered in these theories like choice of single-particle potentials, zero-order states, summation of ring — and ladder— diagrams and occupation probabilities.

RESUMEN

Un posible punto de partida para la construcción de teorías de materia fermiónica infinita o finita lo constituye la suma parcial de la serie perturbativa. Se discuten varios problemas que aparecen en dichas teorías como la selección de potenciales de partícula independiente, los estados de orden cero, la suma de diagramas de anillo y de escalera y las probabilidades de ocupación.

I. INTRODUCTION

Many physical problems involve the calculation of some eigenstate for a given Hamiltonian,

$$H\psi_\alpha = E_\alpha \psi_\alpha \quad . \tag{1}$$

Many-body problems of this kind arise frequently in quantum chemistry[1] and in solid-state[2], quantum fluid[3] or nuclear[4] physics. Throughout this paper I will not discuss the origin of any given Hamiltonian, nor the justification for employing non-relativistic quantum mechanics. I will discuss different methods to obtain approximately some solution of the Schrödinger equation (1). At present, there are three broad classes of computational methods available for this purpose: variational ones, (partially summed) perturbation theory, or stochastic methods. Exact analytic solutions are not available in general for realistic many-body problems. Therefore, stochastic methods currently provide us with the most rigorous results in many-body physics. The Green's Function Monte-Carlo (GFMC) method developed by Kalos and collaborators[5,6,7] has provided us with exact solutions subject to only statistical sampling errors for the ^{4}He atoms fluid[8], model nuclear matter[9], the electron fluid[10], nuclei[11] and atoms[12]. While providing us with exact results stochastic methods are not easily generalized to complex Hamiltonians (1) involving, e.g., exchange forces, tensor forces, nonlocal forces and alike as they occur in nuclear physics. Moreover, many-Fermion systems pose severe difficulties at the present stage. Also stochastic methods frequently are very expensive in terms of computer time.

Variational methods are more flexible than stochastic ones and have been applied extensively to quite complicated nuclear Hamiltonians[13]. In simple cases like the Helium atom they provide us with results of profound accuracy[14]. In genuine many-body problems however two complications arise: firstly, a variational method will only provide us with an upper bound, and it is in general not easy to estimate the distance to the desired Schrödinger eigenvalue, or to obtain a reasonable lower bound. Secondly, in many circumstances the evaluation of the expectation value of the Hamiltonian cannot be done rigorously but has to rely on some approximation scheme. Therefore, one cannot be even sure of having evaluated an upper bound reliably. One exception as regards the latter point is the variational Monte-Carlo method[7] where the expectation value is estimated with only statis-

tical errors. In most integral-equation approaches[15,16] errors due to unavoidable approximations can be estimated.

Perturbational methods in principle are not plagued by any of these problems. They will eventually converge towards true Schrödinger eigenstates. They are even more flexible than the variational methods and may more or less easily be applied to Hamiltonians of arbitrary complexity. By including higher and higher orders the calculations may be carried to any desired accuracy. However, as nice as all this may sound in principle, in practice perturbational methods are the most limited ones because perturbation theory diverges badly in almost all cases of interest, Quantum Chemistry problems[1] being a notable exception. Therefore one has to rely on partial summation schemes summing some classes of contributions to arbitrary order. Of course, this is a very dangerous way to go since it is equivalent to rearranging infinite, divergent series without having any formal proof justifying this rearrangement. In fact the partial summations made in most instances are suggested by physical intuition. One therefore has to be much concerned about convergence properties of the rearranged series – almost all of the rest of this paper will be devoted to this question.

Another drawback of partially summed perturbation methods is the extremely fast increase in numerical effort with the order. Most calculations do already stop at the lowest order, only in few cases has it been possible to proceed one or – in very approximate ways– two orders further.

There is one problem common to all three basic groups of many-body methods: Which eigenstate of the Schrödinger equation (1) will be obtained or approximated? Most frequently one is interested in the "ground state", the lowest energy solution. However, we have to be very careful with this notion since the lowest-energy state will depend on boundary conditions and subsidiary conditions imposed implicitly or explicitly. In order to keep this in mind and be more precise I want to avoid implicit boundary and subsidiary conditions and refer to the "lowest-energy state of a given phase". For example, one might look for the lowest-energy state producing a homogeneous one-body density in space, or the lowest-energy crystalline state, or the lowest-energy pair-condensed state or a spherical nucleus or atom, etc. The absolute

ground state will then be found as the minimum over all phases. This procedure is also more reasonable from a pragmatic point of view since rarely a computational method is able to move between phases, i.e., a calculation started from phase A will under almost any circumstances not be able to produce the lowest-energy state of phase B, though that might be the true absolute ground state.

In section II I will briefly review the Coupled-Cluster or exp(S) method being a very concise and convenient summation of perturbation theory free of approximations. Various subsections will be devoted to current problems in partially summed perturbation theory, namely the choice of zero-order states – a question closely associated with the phase problem mentioned in the last paragraph– the choice of single-particle potentials, and the summation of various classes of Goldstone diagrams corresponding to specific physical processes. The discussion is summarized in section III.

II. PARTIALLY SUMMED PERTURBATION SERIES

A. *The Coupled-Cluster method*

In order to easily manipulate infinite perturbation series it has been found convenient[17,18] to express the desired Schrödinger-eigenfunction in terms of so-called cluster amplitudes S_n,

$$\Psi = \exp\left(\sum_{n=1}^{A} S_n\right) \Phi , \tag{2}$$

where A is the number of particles in the system.

Equation (2) expresses the exact state as some operator applied to a zero-order state Φ which must satisfy

$$\langle \Phi | \Psi \rangle \neq 0 , \quad \langle \Phi | \Phi \rangle = 1 \tag{3}$$

and for fermions in general will be a determinant.

The cluster amplitudes S_n describe the linked or correlated excitation of a n-particle n-hole state with respect to the zero-order state Φ,

$$S_n \Phi = \Phi_{np\ nh} \tag{4}$$

Power-series expansion of the exponential in Eq.(2) produces the remaining particle-hole excited states being composed of two of more independent excitations each involving fewer bodies, e.g.,

$$S_n S_m \Phi = \Phi_{(n+m)p(n+m)h} \quad , \tag{5}$$

$$\Psi = (1 + S_1 + S_2 + S_3 + \ldots + 1/2\, S_1 S_2 + 1/2\, S_2^2 + \ldots + 1/6\, S_2^3 + \ldots)\Phi \tag{6}$$

The expansion (2) or equivalently (6) is seen to express the exact wavefunction as a superposition of the zero-order state and all possible particle-hole excited states with respect to the same, that is, nothing else but an expansion into a complete system of orthonormal functions. The introduction of the exponential form is a concise way to implement the linked-cluster theorem[19]. The wording used here is strongly influenced by the Goldstone diagram expansion[19].

The Coupled-Cluster (CC) method has been described extensively in the literature[17,18,20] including several review papers[18,20,21]. Equation (2) essentially constitutes a transformation of unknowns: instead of determining the A-body wave-function Ψ we now have to determine the set of cluster amplitudes S_n, which are two completely equivalent representations of the same state. In order to obtain the cluster amplitudes we have to use the Schrödinger equation,

$$H \exp(S)|\Phi\rangle = E \exp(S)|\Phi\rangle \quad , \tag{7a}$$

$$S = \sum_{n=1}^{A} S_n \tag{7b}$$

This equation will be multiplied from the left with $\exp(-S)$ and projected onto the complete set of determinants made up from the zero-order state $\langle\Phi|$ and its particle-hole excited states $\langle\Phi_{np\,nh}|$:

$$\langle\Phi|e^{-S}He^{S}|\Phi\rangle = E\langle\Phi|e^{-S}e^{S}|\Phi\rangle = E \quad , \tag{8a}$$

$$\langle\Phi_{npnh}|e^{-S}He^{S}|\Phi\rangle = E\langle\Phi_{npnh}|e^{-S}e^{S}|\Phi\rangle = 0 \ . \tag{8b}$$

While Eq.(8a) is an explicit expression for the energy in terms of the cluster amplitudes S_n the A Eqs.(8b), n=1, ... A, may be used to determine the A unknowns $S_1, \ldots, S_A$. One of the Eqs.(8b) will be referred to as the n-body equation or the equation for S_n. Explicit forms for the equations may be found in Refs. 18, 20, 21, 22. Unfortunately, the equations turn out to be nonlinear and coupled with each other. However, if we assume that the hamiltonian contains only one- and two-body operators, kinetic energy and a two-body interaction for example,

$$H = T + V = \sum_{i=1}^{A} \frac{p_i^2}{2m} + \sum_{i<j}^{A} v_{ij} \tag{9}$$

matters simplify since the equation for S_n will involve only $S_1, S_2, \ldots,$ up to S_{n+2},

$$\begin{aligned}
&X_0\,[S_1, S_2] &&= E\ ,\\
&X_1\,[S_1, S_2, S_3] &&= 0\ ,\\
&X_2\,[S_1, S_2, S_3, S_4] &&= 0\ ,\\
&X_3\,[S_1, S_2, S_3, S_4, S_5] &&= 0\ ,\\
&X_4\,[S_1, S_2, S_3, S_4, S_5, S_6] &&= 0\ ,\\
&\vdots && \vdots\\
&X_A\,[S_1, S_2, S_3, \ldots, S_A] &&= 0\ ,
\end{aligned} \tag{10}$$

where X_n denotes the functional relation between its arguments, the n-body equation.

Since we have not invoked any approximation, the system of equations (10) is equivalent to the Schrödinger equation (1). It turns out, and I will discuss below, that iterative solution of Eqs.(10) will produce the perturbation series or, upon selection of specific paths of iteration through the equations, any desired partial summation scheme.

In order to discuss the Coupled-Cluster equations (10) in more detail it is convenient to use a graphical notation in analogy to Goldstone diagrams. Lines with arrows directed downwards or indices ν will represent states occupied in the zero-order state or holes, while

lines with arrows directed upwards or indices ρ will denote unoccupied or particles states. The amplitudes S_n will be denoted by blobs being entered by n hole lines and being left by n particle lines, i.e., a creation of linked n-particle n-hole excitation. The potential is denoted by a dashed horizontal line. A solid horizontal line denotes an energy denominator, that is the difference between the particle and hole energies for the particle and hole lines it crosses.

With this notation, the most relevant parts of the two-body equation, the equation from which S_2 is to be determined, is shown in Fig.1. Consider for the moment just the first three terms, (a) to (c), as an iterative scheme to determine S_2. In the first iteration we find

$$S_2 = -(Q_2/e_2)\, v \;; \tag{11}$$

the first-order perturbation theory result for the wavefunction change. Inserted into the energy expression,

$$E = E_{HF} + \langle \Phi | v S_2 | \Phi \rangle \quad , \tag{12}$$

this is seen to produce the second-order perturbation correction to the energy. There is no first-order contribution since we assume the unperturbed state $|\Phi\rangle$ to be the Hartree-Fock (HF) solution.

Further iteration of Fig. 1(a) to (c) will produce an increasing number of interactions between the particles, Fig.2. In fact the equation we are solving (formally) iteratively is just the familiar Bethe-Goldstone equation[20]:

$$e_2 S_2 = -Q_2\, v(1 + S_2) \quad . \tag{13}$$

In Eqs. (11) to (13), e_2 denotes a two-body energy denominator, and Q_2 a two-body Pauli projection operator which takes care that the particle lines in Figs. 1 and 2 really are particles.

In this approximation, our two-body equation just yields the sum of all two-body scattering processes between a pair of particles, summed to infinite order of perturbation theory. This is the first case we encounter where a partial summation has been performed. There are many contributions to the energy of third, fourth,..., order in the

energy which have been neglected so far, for example all of the terms resulting from the wavefunction amplitudes of Fig.3 when inserted into the energy expression Eq.(12).

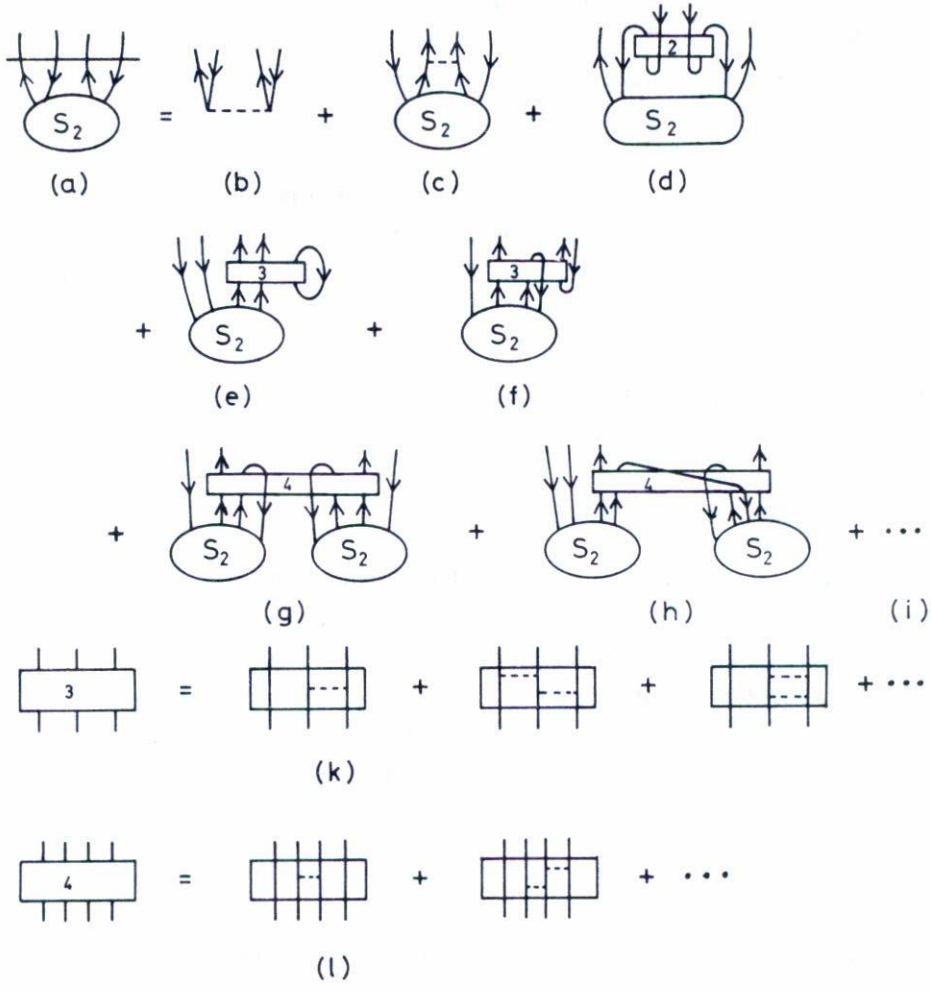

Fig. 1 Equation for the two-particle two-hole excitation amplitude S_2 in diagrammatic form. The "3"- and "4"-body boxes denote the three- and four-body Bethe-Faddeev summations, i.e., the sum of ladder diagrams.

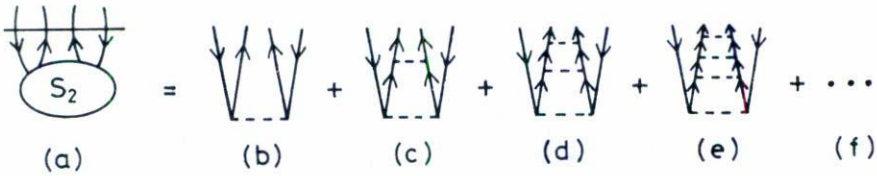

Fig.2 Lowest order approximation to S_2 for the short-range forces. This sum of two-body ladder diagrams is obtained from the Bethe-Goldstone equation, terms (a) to (c) of Fig.1.

It is justified to take along a second-order contribution like Fig.2(c) and at the same time omit a contribution like Fig.3(a) of the same order? Fortunately, this question can be answered unambigously due to the presence of certain singularities in the equations for certain classes of interaction potentials v. If the interaction v has a hard-core, i.e., if it is infinitely repulsive over a finite interval, one must keep together all the terms of Fig.2 any of which does not exist (is equal to infinity) but the sum of which does exist and even provides correctly the leading term of the low-density expansion[23] of the total energy Eq.(12). The presence of the hard-core forces us to deviate from order-by-order perturbation theory and keep together certain classes of diagrams to all orders. Simultaneously, these classes of diagrams acquire a physical "meaning": the diagrams of Fig.2 are said to represent the multiple-scattering series for the two particles involved.

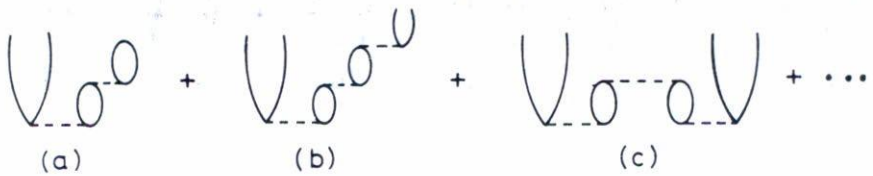

Fig.3 Lowest order approximation to S_2 for long-range forces. This sum of ring diagrams is obtained from the RPA-equation, terms (a), (b), (f) and (g) of Fig.1 together with the lowest-order approximations Fig.1 (k) and (l).

As another extreme let me discuss the Coulomb potential. Because of its long range, in an infinite system (e.g., a metal) taking v to be 1/r leads to another singularity. The individual terms of Fig.2, as well as their sum, are well behaved since we do not have a hard-core, but the diagrams of Fig.3 now do not exist, but only their sum. This is just the familiar statement that in an infinite Coulomb system the sum of ring diagrams must be kept together, and the physical meaning acquired by this partial summation is the "screening" of the long-range Coulomb force due to collective processes. Like the ladder diagrams in the hard-core case, the sum of ring diagrams furnishes exact leading-order terms for the energy and other quantities in the Coulomb case[24,25].

Since the leading terms of the two-body equation seem to produce just the ladder diagrams and not the rings, one might believe that the Coupled-Cluster method is especially adapted to treat short-range forces. This, however, is <u>not</u> true – it is only a consequence of

our notation that ladders are recovered more easily than rings. In fact, upon iteration Figs. 1(f) and 1(g) will produce all the ring diagrams if we replace the "3" and "4"-body boxes (to be discussed below) by just one interaction v-their lowest order- in a suitable manner [Fig. 1(k), 1(l)].

The Coupled-Cluster equations, as is obvious from the preceeding discussion, have the appealing feature that even in a low-order approximation, like considering S_2 only, they do contain the correct lowest-order approximations for two completely adverse problems: the (short-range) hard-core problem as well as the (long-range) Coulomb problem. In fact, the two-body equation Fig. 1 as it drops out by purely formal manipulations of the Schrödinger equation (8b) turns out to embody the most important physics of these two quite different many-body problems and is able to describe two-body short-range correlations as well as long-range screening. The partial summations of perturbation theory suggested by this equation are just those required in order to avoid singularities in extreme cases.

Since most of the problems I want to discuss below concern many-body systems interacting via short-range potentials, the form Fig.1 for the two-body equation is the useful one. In Coulombic problems one would choose to write down the equation differently, that is employing nothing but a different notation and a different grouping of terms [21,25].

B. *Zero-order States*

Before talking about particles and holes one should specify what these single-particle (s.p.) states are to be. The very Ansatz for the wavefunction, Eq.(2), assumes a zero-order or reference state Φ to be given which for fermions usually is taken to be a determinant. In the present section I want to address the question what the significance of choosing one or other prescription for this state is.

The full, presumably exact, wavefunction Ψ is built up from Φ by means of npnh-excitation operators S_n. The idea of a practical calculation to be carried out is, of course, to truncate the coupled set of equations (10) for the S_n and calculate only a small, finite subset up to S_N and neglect all S_m, $m > N$. In order for this scheme to work one should at least be sure that the S_n will not grow with n in which case any truncation would be disastrous. In some sense, for any approximation

scheme within the context of the Ansatz equation (2) the S_n must be "small". In other words, the unperturbed state Φ must be close to the true state Ψ in order for approximate schemes to work. This is already suggested by Eq.(3): if the unperturbed and exact states are orthogonal, even the exact method does not work! In this sense Coupled-Cluster theory is akin to perturbational methods. In spite of the partial summations made it is still required that the solution be not too far from the zero-order state.

Let me discuss some examples. In an infinite system there exist essentially four different phases: fluid, solid, superfluid, and clustered. In the case of the Heliums these phases are familiar, at least the first three. The clustered phase is thought to consist of droplets (of several ^{4}He atoms, say) forming a (low-density) fluid.

At a given density, we do not know a priori which of these phases will be lowest in energy. On the contrary we might be tempted to calculate the equation-of-state for fluid Helium-3 as a function of density ignoring the phase boundaries. For this problem, since we expect the true, fully interacting wavefunction to produce a constant number density in space it is reasonable to use plane waves as s.p. states to built a determinant Φ from. In fact, this is precisely what has been used in most calculations so far[16,26].

On the other hand when interested in the properties of solid Helium-3 we would <u>not</u> use plane waves in zero order since localization of particles at lattice sites is believed to be an essential feature of solids which we should not like to miss, even in zeroth order. In fact, we would use localized s.p. orbitals[27] centered around lattice sites for this problem to build a determinant from. This intuitive, physical choice in each of the two cases will lead to "reasonable" magnitudes for the correlation effects (although it should be noted at this point that the Helium-3 fluid as well as the solid are too strongly correlated systems to be treated by the Coupled-Cluster method at all to our current knowledge). Our choice of reference states allows us now to calculate the energy of <u>two</u> phases at the same density. Neither calculation exhibits instability against the other phase even if the other phase is significantly lower in energy.

In other words, a method like the Coupled-Cluesters in practice

is not able to move from one phase to another. Given a zero-order state Φ, the solution Ψ of the Schrödinger equation approximated will be one of the same symmetry —not necessarily the ground state. Similar statements hold true for almost any other method, in particular for variational methods, but not in general for the Green-Function-Monte-Carlo method.

If one would try to approximate a solid starting from the fluid plane-wave determinant it is rather obvious that one would get very large S_n amplitudes. The solid-like structure implies long-range, many-body correlations which if not embodied within the reference state must be build up by the S_n.

A similar situation exists if one is interested in the superfluid state. It is necessary to use as reference state one which already is superfluid, like a BCS state[28]. If one tries to describe a superfluid state starting from a normal fluid one, divergent S_n amplitudes result[28]. The clustered state will exhibit the same problems as discussed above for fluid/solid states. Within a given symmetry it has been found useful to use as occupied s.p. states those resulting from a (symmetry-restricted) HF or generalized HF[18] scheme. The latter one results from requiring $S_1 = 0$.

The essence of all the above discussion is that it is not possible to ask of most many-body methods, in particular the Coupled-Cluster method, "Given some reference state, produce the ground state". The only question allowed and possible to answer is "Given some reference state, produce some eigenstate of the Schrödinger equation". It is then general experience that the state produced will be the one for which the overlap $\langle \Phi | \Psi \rangle$ is maximal, or, if we wish to keep $\langle \Phi | \Phi \rangle = 1$, the overlap $\langle \Psi | \Psi \rangle$ is minimal, both expressing the fact that the eigenstate found is the one "closest" to the unperturbed state. It is then a consequence that the eigenstate found will be of the same phase as the zero-order state. It may be hoped that one will obtain the lowest-energy state of that phase. The only way to produce the absolute ground state is to calculate separately for all possible phases and take the minimum of the energy.

This last problem unfortunately is by no means trivial since it requires knowledge about all possible phases. In the Helium-3 problem,

for example, only the fluid, solid, and superfluid phases are well-known. At small densities, however, significantly below the fluid saturation density, the clustered phase (in particular, just one huge droplet) is to be expected to be lowest in energy which is not generally well recognized. It is therefore important to search for possible other phases[29].

Another interesting observation may be made when employing different zero-order states. Using the fluid/solid example of above, one calculates saturation (energy vs. density) curves qualitatively shown in Fig. 4(a). At any density there exist two different eigenstates of the Schrödinger equation having different symmetry properties. However, it is very well known[30] that Schrödinger eigenvalues cannot cross. Therefore, the situation actually is like in Fig.4(b), i.e., there exists an "avoided" level crossing, a situation which in several known cases leads to divergencies in perturbation theories[31]. The fact that one does not realize the least bit of trouble in actual Helium calculations demonstrates nicely the ability of approximate methods to run straight across the avoided crossing in Fig.4(b) without experiencing any divergencies. The reason for this ability is the great difference in structure between the two states involved because of which there is no coupling at all between them, and one may be considered without any reference to the other. It is not clear in how far the fluid/solid situation is similar to problems in nuclear physics[32].

C. *Single-particle potentials*

In section II.A, I introduced an energy denominator made up from s.p. energy differences,

$$e_n = \sum_{k=1}^{n} (\varepsilon_{\rho_k} - \varepsilon_{\nu_k}) \quad , \tag{14}$$

for the n-body case. There has been some discussion in the literature about what these s.p. energies should be[33]. Considering the exact two-body equation, Fig. 1, there arises no problem of this sort. If someone does not want to have certain terms in the s.p. denominators, that is on the left hand side of the equation, he may easily put those terms on the right hand side of the equation and thereby get rid of them, or vice versa. The organization of terms in an exact equation should not matter. Problems

arise if approximations are to be introduced. In that case, grouping together of some terms usually is meant to suggest as approximation to neglect the whole group of terms, and not only part of the group.

The s.p. energies consist of a kinetic and eventually potential term,

$$\varepsilon_\alpha = T_\alpha + U_\alpha \quad , \tag{15}$$

diagrammatically shown in Fig.5. The grouping together of terms used in Fig.1 corresponds to having only the terms outside the brackets in the energy denominator. The terms in brackets are contained in Figs.1(e) and (h), i.e., on the right hand side. In other words, we suggest to use a s.p. potential for the holes created self-consistently [Figs.5(b), (c)] but kinetic energy only for the particles [Fig.5(f)]. The potential energy for the particles, Figs. 5(g) to 5(k), is taken together with some other contributions in Figs. 1(e), (h).

In order to justify this grouping and resulting approximation schemes to be discussed below let me again discuss two extreme cases, the hard-core gas and the Coulomb fluid.

For the Coulomb fluid, one would <u>not</u> use the grouping as described in the last paragraph. For the long-range Coulomb force, small-momentum excitations just around the Fermi surface are of great importance. By analytic continuation arguments[34] it may be shown that the s.p. energy and thus potential must be continuous at the Fermi surface. Therefore, one is forced to use exactly the same approximations for the particle as well as the hole potential, e.g., kinetic energy only for <u>both</u>, or kinetic energy plus HF potentials [Figs. 5(b),(g)] for <u>both</u>, or kinetic energy plus HF potentials plus correlation contributions [Figs.5(c),(h)] for <u>both</u>. Whatever is not taken into the s.p. energies will be found on the right-hand side of Fig.1, and approximation schemes may be discussed neglecting some or all of the remaining contributions.

For the hard-core gas, we have to keep together the multiple-scattering series in order to avoid infinities. The HF potentials, Figs.5(b),(g) do not make any sense by themselves in this case, Fig.5(b) only together with Fig.5(c) is finite, and similarly Fig.5(g) has to be kept together with Figs.5(i),(k),(l). At first sight using precisely

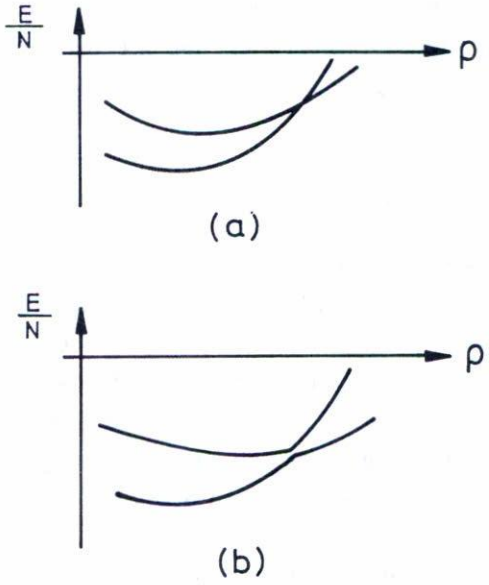

Fig.4 Schematic equations of state in a two-phase region.
(a) Two independent calculations producing the two equations of state for the two phases.
(b) Schrödinger eigenvalues obeying the non-crossing rule.

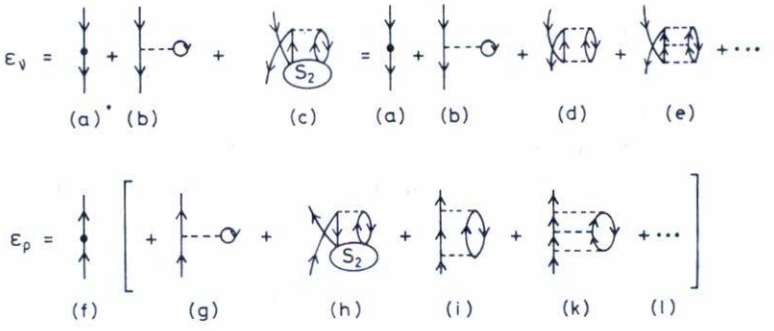

Fig.5 Single-particle energies. The dot denotes kinetic energy.
(a) to (e), for hole states.
(f) to (l), for particle states. The diagrams in brackets must be omitted in the case of short-range forces.

these terms for the s.p. potentials seems to be perfectly reasonable. If a particle is moving inside a many-body medium it will acquire a self-energy due to its interactions with the other particles around, which is precisely the physical interpretation of Figs.5(g), (i), (k), (l). This argument would be perfectly right if there existed some particle moving through some medium, like in the case of an optical potential. In the ground-state problem, however, there never occurs just one particle inside the medium. In order to create a particle we must have some two-body collision taking place creating a pair, i.e., two particles moving inside the medium. This fact invalidates the previous discussion. Consider Fig.6 where the situation is shown in some detail. Figure 6(a) shows the process of Fig.5(k) in context. One of the two particles excited in some two-body process interacts with a third particle. However, with a strong short-range force, particles 1 and 2 will always be very closely spatially correlated. The interaction of 2 with 3 via a short-range force also implies a short-range correlation between these two particles. Therefore, also particles 1 and 3 must be close together and it is equally likely that 1 and 3 will interact, like in Fig.6(b), as it is that 2 and 3 will interact, Fig. 6(a). However, while Fig.6(a) could be termed a particle potential, Fig. 6(b) can not: it involves a genuine three-body scattering process. In the presence of short-range forces it is very well known[35] that not only all two-body scattering processes must be considered in their entirity or not at all, but also all three, four, ..., body scattering processes must be considered in their entirity or not at all since they form a diverging series. It is consequently a bad approximation for a short-range force to select out processes like Fig.6(a) to keep and those like Fig. 6(b) to discard which is precisely what one does if one introduces a particle potential energy in a two-body theory. The only admissible "particle potential" is the one retaining all the three-body processes, i.e., Fig.6(c). Of course, one has to solve a three-body equation to get it.

For a short-range force one therefore has two alternatives: either neglect all the potential contributions, i.e., take kinetic energy only for the particle states, or take into account all three-body processes like Fig.6(c) which involves solution of the three-body Bethe-

Faddeev equation[36]. The resulting two-body matrix of Fig.6(c), however, does not have the nice physical interpretation of a one-body particle potential. It definitely is a strongly non-local two-body operator. Therefore, it does not make much sense to put those contributions into an energy denominator. This is why in Fig.1 these terms have been put on the right-hand side of the equation, Fig.1(e), and the energy denominator in Fig.1(a) contains kinetic energy only for the particles. For the holes no corresponding discussion arises since hole states are not spatially correlated.

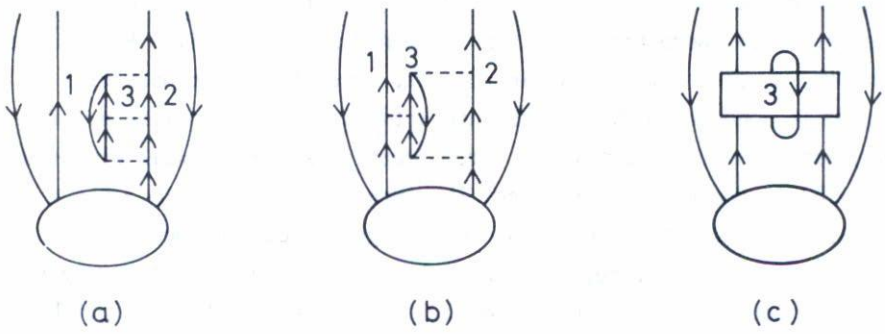

Fig.6 Origin of the Bethe-Faddeev summation, for ladder diagrams.

In any given problem, like nuclear matter for example, the question arises if we are closer to the Coulomb-fluid situation or if we are closer to the hard-core gas situation. In the first case, a potential for particles would be justified, in the second case not. Numerical calculation[22,33], bears out that the situation is somewhere it between. This fact, however, implies that no reliable calculation can be carried out at all without calculating the three-body contributions since these are of the same order of magnitude as those taken into account via a particle potential.

Since one may always add and substract an arbitrary term, one could introduce an arbitrary "model" particle potential into the two-body approximation, and subtract it from the three-body term. If one knew how the three-body term would look in general, this would be a very reasonable procedure. However, in practice there is no general scheme available. In the sense that an arbitrary parameter is introduced

into the theory, one must make sure that the final results do not depend on it. If one therefore chooses the introduce whatever particle potential one likes, one is of course free to do so if this can be shown not to affect the final result. In order to show this, however, one would have to solve a three-body Bethe-Faddeev equation using the stipulated particle potential, and nothing is gained.

D. Rings and ladders

In fact the situation for nuclear matter is even worse than I sketched in the last section. If we want to discuss three-body contributions, then besides Fig.1(e) we also have to discuss Fig.1(f) the lowest order of which are shown in Fig.7. If we close these diagrams on the top with an additional interaction line they are seen to yield ring diagrams for the energy. Iterating Fig.1(f) to all orders will in fact produce all forwardgoing ring diagrams, i.e., the Tamm-Dancoff approximation (TDA).

Let me again consider the two extreme cases of the electron fluid and the hard-core gas. For the electron fluid, the ring diagrams form a diverging series[24] and must be summed in closed form. In this case, Fig.7(a) is the single most important contribution to the two-body equation, Fig.1. This term is much more important than any self-energy term, provided we do not introduce a discontinuous single-particle spectrum at the Fermi surface.

In the hard-core gas, Fig.7(a) by itself again is not meaningful but all two-body processes have to be taken together, i.e., the other two-body scattering terms of Figs.7(b), (c) etc. must be included with Fig.7(a). Then, however, there is precisely the same argument as in the preceding section applying to Figs.7(c),(d): The third particle present must be included in all scattering processes, i.e., we again have to perform a three-body Bethe-Faddeev summation leading to Fig.1(f).

In the intermediate (nuclear matter) situation one is now cought between two arguments: if it is of great importance to have the single-particle spectrum continuous at the Fermi surface because of important low-momentum excitations, then one immediately knows that also contributions like Fig.7 will be important – like in the electron fluid. If the diagrams of Fig.7 are not important, however, than also the con-

tinuity of the s.p. spectrum is very likely at disposition.

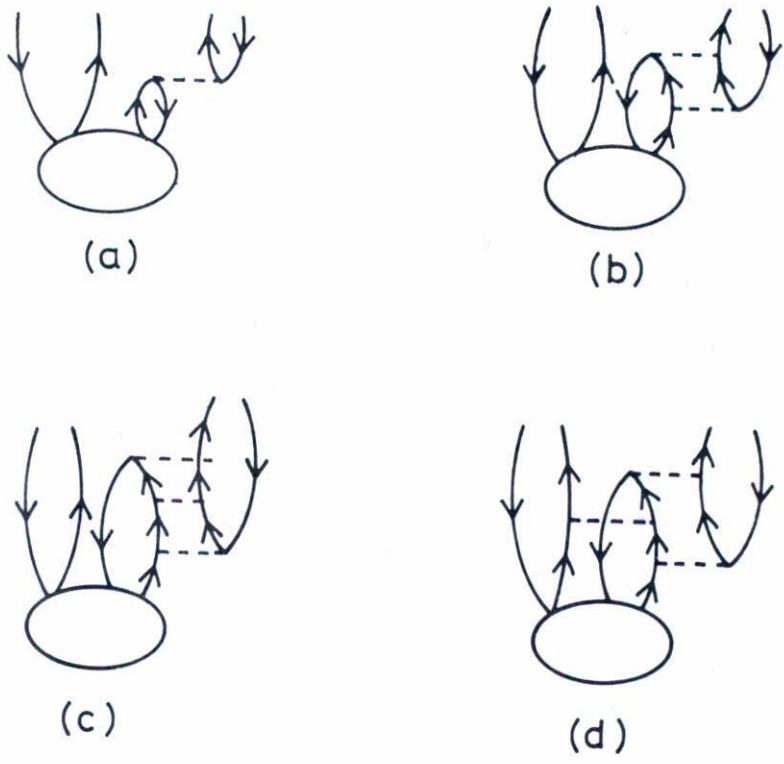

Fig.7 Origin of the Bethe-Faddeev summation, for ring diagrams.

The best way out is of course again to perform the three-body summation and include all these diagrams via Figs.1(e),(f)[22,36].

It should be mentioned that the solution of three-body Bethe-Faddeev solution does not get us rid of the problem completely, but only pushes it one order farther down in the hierarchy of equations, Eq.(10). When solving the three-body equation, no problems remain on the two-body level, Fig.1. However, precisely the same questions are to be answered now when solving for the three-body amplitude: what are the s.p. potentials to be? For the holes things again are obvious. For the particles, however, having one the three closely correlated particles

involved in a collision with a fourth one immediately forces us to consider a four-body problem (Fig.8), i.e., solve the four-body Bethe-Faddeev equation[18,36] and so on. We realize at this point that in truncating the hierarchy of Eqs.(10) we always will face the same kind of problems and eventually will– for a short range force– have to resort to using kinetic energy only for the particles in some n-body equation, the last one we actually consider solving. Numerical calculation[18,22,36] bears out, fortunately, that on the three-body level the choice already does not matter any more: for all practical purposes solving the three-body equation with kinetic energy only allows us to evaluate Figs. 1(e),(f) to sufficient accuracy.

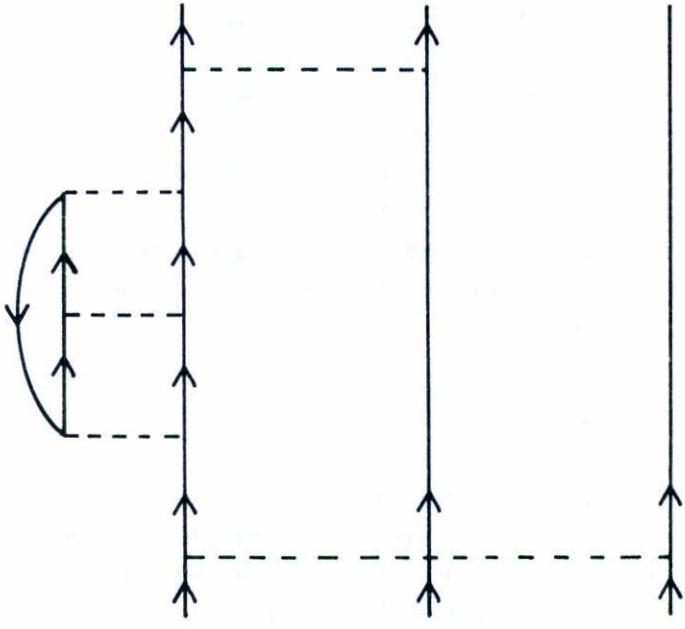

Fig.8 Four-particle scattering resulting when trying to use particle potentials within the three-body Bethe-Faddeev summation.

For the Coulomb problem it is not sufficient to include only the forward-going ring diagrams. One also must include the backward going ones, i.e., the full Random-Phase approximation (RPA). This is

done via Fig.1(g). This class of processes is seen to involve a four-body Bethe-Faddeev summation as well in the hard-core case (short-range forces). However, fortunately it has been observed many times[18,22,36] that these contributions for short-range forces are cancelled to very good accuracy by those of Fig.1(h). Since it is not possible to solve the four-body Bethe-Faddeev equation with presently methods the best approximation is to leave out these terms in the case of short-range forces.

E. *Occupation probabilities*

In various places there occur interactions of particles or holes with "the medium", i.e., all the occupied states, denoted graphically by elements like Fig.9(a). It has been argued[37] that these terms must be modified since not all the occupied states are occupied all the time. In fact, the very form of the exponential ansatz, Eqs.(2) and (6) shows that while we are looking at some S_2 matrix element and the equation for it at other places within our many-body system other excitation processes depleting the Fermi sea take place. Diagrammatically, this consideration leads to terms like Fig.9(b) which are of opposite sign than Fig.9(a). Approximately, when some term including process Fig.9(a) has the value A, the same term replacing Fig.9(a) by Fig.9(b) has the value $A(-\kappa)$, with

$$\kappa = \frac{1}{2}\frac{1}{N}\sum_{\nu_1\nu_2} \langle \nu_1\nu_2 | S_2^+ \; S_2 | \; \nu_1\nu_2 \rangle \tag{16}$$

The sum of both processes is therefore given by $A(1-\kappa)$. This expression has a nice physical interpretation. κ, Eq.(16), is the probability for any hole state to be depleted, i.e., for the particle normally occupying it to be excited, since S_2 is the amplitude for such an excitation process. Any term involving summations over occupied states is therefore reduced by the factor $(1-\kappa)$ being the probability for a hole state to be actually occupied.

The most prominent places where summations over occupied states occur are the hole- and particle-potentials, Figs.9(c),(d) show the corresponding renormalizations [to Figs.5(b),(c) and 6(c)]. In a two-body approximation one would only have Fig.9(c) but not Fig.9(d)

since the particle potentials for short-range forces come in only from the three-body equation. In this case, the hole potential is significantly reduced by the factor $(1-\kappa)$. The energy denominators become smaller, therefore, resulting in additional attraction.

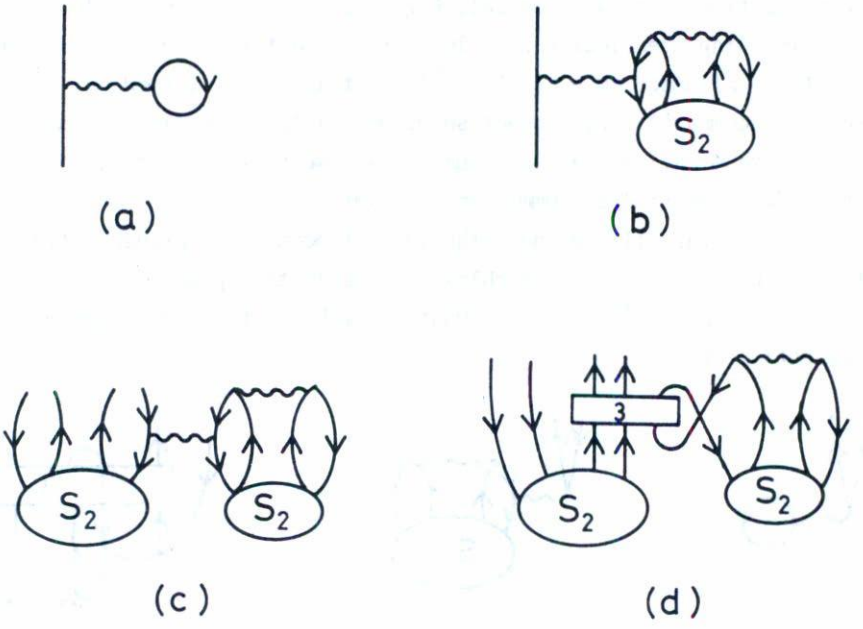

Fig.9 Origin of occupation probability insertions.
(a) interaction with occupied states;
(b) subtraction from (a) due to depletion of occupied states;
(c) same as (b), in the two-body occupied state energy denominator.
(d) same as (b), in the "particle potential".

Most of this is quite spurious, however. Upon inclusion of particle potentials via three-body processes, Fig.1(e), one also has the corresponding renormalization, Fig.9(d). The energy denominators remain almost unchanged by the occupation probability renormalization now since the particle potential is equivalently reduced. Moreover, there are some combinatorial factors coming in [38] which reduce the renormalization for the hole potential. In spite of the hole potential being stronger than the particle potential, the renormalizations there-

fore cancel to a high degree. In the nuclear matter problem occupation probabilities are not very important, therefore[22].

Another place where occupation probabilities have been thought to be important is the self-consistent single-particle potential to be used in the one-body, or generalized Hartree-Fock equation[39]. The renormalization to this potential, Fig.10(a), is given in Fig.10(b). This term being identically zero in infinite matter has had an additional saturating influence on nuclei[18,39]. Lately it has turned out[40], however, by comparison with exact solutions of the Schrödinger equation[11], that this renormalization contribution is essentially cancelled by its three-body Bethe-Faddeev summation, Fig.10(c).

Taking all together, the idea of occupation probabilities is not a useful one in nuclear problems. Exactly the opposite is true in many-Boson problems[41] where occupation probabilities do contribute in an essential manner.

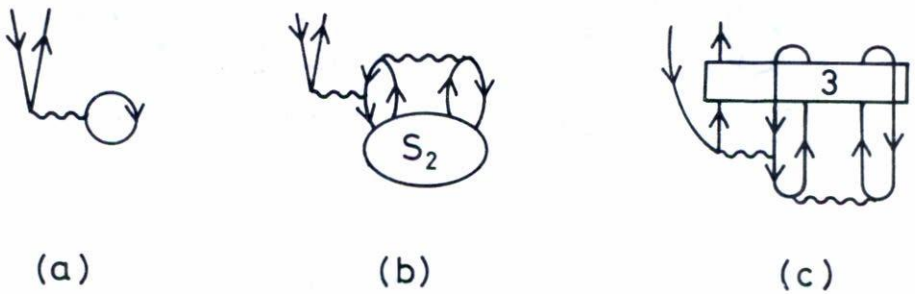

Fig.10 Ocupation probability renormalization of the particle-hole potential.
(a) lowest order particle-hole potential
(b) depletion subtraction from (a)
(c) Faddeev summation cancelling (b)

F. *The hole-line expansion*

Throughout the previous sections I used the Coupled-Cluster formulation of many-body theory. Historically, in the nuclear matter problem the hole-line expansion[20,22] has been used extensively. The hole-line expansion is easily recovered from the Coupled-Cluster scheme[22,42] by iterating the equations. Consider Fig.1. Iterating terms Figs.1(a),(b),(c) produces the Brueckner reaction matrix G or K,

or the two-hole-line approximation. By iterating in addition Figs.1(d), 1(e) and 1(f) once we obtain terms involving an additional hole line, i.e., three-hole-line terms. Upon inspection these are found to be all the three-hole-line terms[20]. Iterating these terms another time yields some four-hole line terms, other four-hole line terms are recovered by iterating Figs.1(g),(h),(i). In general, in order to recover the full n-hole-line approximation, we have to take into account some terms of the n-body equation iterated once, of the (n-1)-body equation iterated twice, ..., of the 2-body equation iterated (n-1)-times.

The hole-line expansion is essentially a low-density expansion. In this sense it is related to the Coupled-Cluster theory which relies on n-body clusters becoming small for large n, which also will hold true only for not-too-large densities. It is therefore not too surprising that both theories yield quite similar results[22].

It is to be noted, however, that the n-body Coupled-Cluster theory always is more comprehensive than the n-hole-line approximation. It contains all the n-hole-line diagrams plus a large number of self-consistent iterations, usually building a whole class of diagrams upon any single hole-line diagram. Consider the three-hole-line approximation, for example. It will contain just the lowest-order ring diagram, Fig.11(a). The three-body Coupled-Cluster approximation, however, will iterate Fig.1 to all orders thereby producing all the forward going ring diagrams of Fig.11(b),(c), etc. Similar observations hold true in a great number of other places.

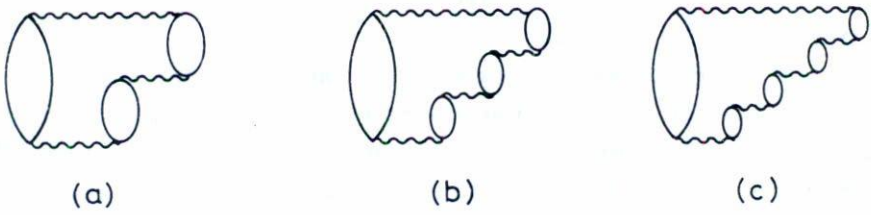

Fig.11 Ring diagram contributions to the energy.

Though it does not occur in practice, i.e., for existing nuclear force models, Coupled-Cluster theory is capable to deal with much more complicated situations than the hole-line expansion. If there were a strong spin-isospin mode in nuclear matter, i.e., if we were close to a pion condensation threshold, long-range correlations would build up due to the processes Fig.11 – like the plasmon mode is build up in the electron fluid. This would lead to a divergent hole-line expansion, but could very well be treated by the three-body version of Coupled-Cluster theory. The fact that there is no indication of divergence in the hole-line expansion may therefore also be taken as an indication that there is no threshold for pion condensation anywhere near the densities considered so far, i.e., up to twice nuclear density.

Detailed comparisons of hole-line and Coupled-Cluster approximations may be found in Refs. 18, 20, 22, 42.

III. SUMMARY

Partially summed perturbation series are one important tool in the description of many-fermion ground states. They offer great flexibility and adaptability to any ground-state problem. Complicated nuclear hamiltonians do not create the significant problems they introduce into variational[13-16] or stochastic[5-12] schemes. They do suffer, however, from the lack of any formal proof of convergence. One has to rely therefore on physical arguments as to why some approximation scheme should be reasonable or preferrable above some other, besides numerical investigations of convergence properties and quantitative comparison with other theories, like variational or stochastic ones, in their range of applicability.

Numerical results show that the Coupled-Cluster as well as Brueckner-Bethe (hole-line expansion) methods are in agreement with each other as well as any other reliable calculation put forward so far[22,40]. The previous sections have tried to explain what the physical reasons behind this success are, and why for different hamiltonians like the Coulomb one different approximation schemes have to be used. This comparison teaches us that nuclear forces are sufficiently short-ranged to necessitate the ordering scheme according to the number of interacting

bodies, i.e., the introduction of n-body Bethe-Faddeev summations.

There are intriguing problems, however, which up to now cannot be treated by this class of methods, namely the phases of liquid ^{3}He. In spite of the simple central force even the variational schemes so far have failed to come close to experimental results for the liquid saturation curve[43]. This failure is due to the strong many-body correlations introduced by the huge repulsive core present in the interaction, and the strong state-dependence of these correlations. Though the Coupled-Cluster theory would perfectly be capable of dealing with the state-dependence, the strength of the repulsive core and the high density of the system lead to slow a convergence in cluster amplitudes, i.e., one seems to be forced to solve three-, four-, maybe even five-body equations. It may be hoped that these difficulties could be overcome by the Correlated Coupled-Cluster method[44], a joining of variational and Coupled-Cluster schemes.

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