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Compact-Cluster Expansion for the Nuclear Many-Body Problem

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Bethe's treatment of three-body clusters is extended to the entire linked-cluster perturbation series. The result is a completely rearranged expansion in terms of "compact clusters." The spatial correlations within these terms are all of quite short range. As a direct consequence, each of these new compact-cluster terms is proportional to $\kappa^{h'-1}$, where h' is the number of momenta inside the Fermi sea which can be summed independently after allowing for momentum conservation. The "small parameter" of the expansion is $\kappa=\rho\int|\zeta|^2 d\tau$, where ρ is the ordinary nuclear density and $\zeta=\phi-\psi_{BG}$ is the "wound" in the correlated two-body (Bethe-Goldstone) wave function. In nuclear matter this κ is of order 10%. This result requires that the single-particle potentials be defined in terms of a certain subset of all the self-energy insertions. The allowed insertions are those which can be evaluated entirely on the energy shell, by means of a "generalized time-ordering" factorization. The totality of these insertions is said to constitute an "on-energy-shell mass operator" M^{on}. The resulting occupied-state potentials are quantitatively very similar to those of most previous versions of nuclear-matter theory. However, the present intermediate-state potentials are small enough (being only of order +1 MeV) to be safely ignored in practical calculations. This simplification is offset by the need for a separate calculation of the three-body clusters. These single-particle potentials are "physically meaningful" in the sense that they lead to an optimum treatment of the short-range correlations. The bulk properties of nuclear systems are determined almost entirely by these short-range correlations. It is therefore proposed that similar potentials be used in a many-body theory of finite nuclei. True occupation numbers occur in a simple and natural way throughout the entire expansion. The formal and practical consequences of this feature are carefully examined. It is argued that this is significant for a theory of finite nuclei. Comparisons are made with several different "renormalized" formulations of quantum statistical mechanics, and also with the Green's-function theory of nuclear matter. The present formulation tends to artificially suppress the long-range correlations (e.g., pairing correlations) between particles near the Fermi surface. This defect can be eliminated by using a degenerate analog of the Goldstone expansion.

I. INTRODUCTION

TWO developments in the Brueckner-Bethe-Goldstone theory of nuclear matter have emphasized the need for a more complete understanding of the higher order terms in this theory. On the one hand, attempts to extend this theory to actual nuclei have focused attention on the self-energy problem. Several authors[1–6] have shown that the higher order terms which have been associated with the "rearrangement energy" play an important role in determining the saturation properties of actual nuclei. On the other hand, Bethe's improved treatment of three-body clusters,[7] to *all* orders of perturbation theory, represents a radical departure from previous ideas about the convergence of the theory. This treatment suggests the possibility of systematically rearranging the *entire* perturbation series, in such a way that a rapid rate of convergence can be seen directly from the structure of the new series. Such a "renormalized" perturbation series should make the theory of nuclear matter more accurate and more convincing than previously. It may also lead to more confidence in extensions of the theory to liquid He^3, because there the practical problems of convergence are much more severe.[8] The main purpose of this paper

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[1] K. A. Brueckner and D. T. Goldman, Phys. Rev. **116**, 424 (1959).
[2] K. A. Brueckner, A. M. Lockett, and M. Rotenberg, Phys. Rev. **121**, 255 (1961).
[3] H. S. Köhler, Nucl. Phys. **32**, 661 (1962).
[4] K. S. Masterson, Jr., and A. M. Lockett, Phys. Rev. **129**, 776 (1963).
[5] B. H. Brandow, Compt. Rend. Congr. Intern. Phys. Nucl. Paris **2**, 295 (1964).
[6] H. S. Köhler, Phys. Rev. **137**, B1145; **138**, B831 (1965).
[7] H. A. Bethe, Phys. Rev. **138**, B804 (1965). For an alternative treatment, see also S. A. Moszkowski, Phys. Rev. **140**, B283 (1965).
[8] K. A. Brueckner and J. L. Gammel, Phys. Rev. **109**, 1040 (1958).

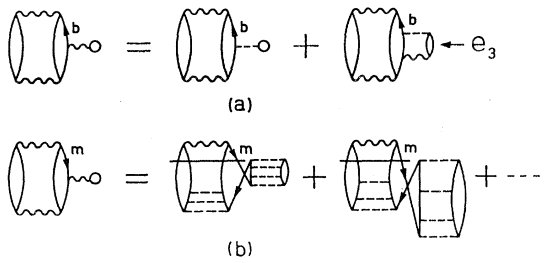

FIG. 1. Examples of interaction (a) off the energy shell, and (b) on the energy shell.

is to present a renormalized perturbation theory of this character.

We believe that this expansion can also provide a satisfactory formal description of the shell-model potential. A brief justification for this view will be given here. Most of our discussion of the problems raised by the finite geometry will, however, be reserved for a future paper.

The present rearranged expansion can be extended to open-shell nuclei, and to systems with pairing and random-phase correlations, by performing similar partial summations in the context of the degenerate linked-cluster formalism.[9–13] In principle, this approach should therefore provide a *quantitative* theoretical basis for Landau's phenomenological theory of a Fermi liquid,[14] insofar as this applies to nuclear matter and liquid He^3. Suitable degenerate analogues of the present expansion will be discussed in a later paper. We have found that the important subjects of the rearrangement energy and the optical potential cannot be dealt with adequately without invoking this degenerate formalism, so these topics will not be discussed here.

A number of other many-body formalisms were considered during the course of this investigation. These included the Green's-function method as well as the perturbation methods of quantum statistical mechanics. Comparisons are made with these other formalisms in order to illustrate and defend the special features of the present scheme. We believe that this is the most satisfactory method for the nuclear many-body problem. This is because the present method optimizes the treatment of the short-range few-body correlations. These are by far the most important correlations for the bulk properties of nuclear systems. As mentioned above, other types of correlations can be handled by using degenerate analogues of this theory.

[9] C. Bloch and J. Horowitz, Nucl. Phys. **8**, 91 (1958).
[10] B. D. Day, Ph.D. thesis, Cornell University, 1964 (unpublished). This study is quite similar to Ref. 9, both as to methods and results, although the work was done quite independently.
[11] T. Morita, Progr. Theoret. Phys. (Kyoto) **29**, 351 (1963).
[12] B. H. Brandow, in Proceedings of the International School of Physics "Enrico Fermi," Course 36, Varenna, 1965 (to be published).
[13] B. H. Brandow, Rev. Mod. Phys. (to be published). This paper will be referred to as LCE.
[14] L. D. Landau, Zh. Eksperim. i Teor. Fiz. **30**, 1058 (1956); **32**, 59 (1957); **35**, 97 (1958) [English transls.: Soviet Phys.—JETP **3**, 920 (1957); **5**, 101 (1957); **8**, 70 (1959)].

The entire rearranged expansion exhibits some interesting formal relations which are summarized by an unusual variational principle. The physical significance of this variational principle is explored.

There are three basic ideas in the present formulation, and these can all be expressed quite simply. These are (i) *compact clusters*, (ii) *on-energy-shell insertions*, and (iii) *true occupation probabilities*. These concepts are introduced in Secs. II, III, and IV. The physical motivations for this formulation are discussed in Sec. V. The most interesting practical consequence is the rapid initial rate of convergence. This is characterized by a "small parameter" κ, which is numerically of order 10% for nuclear matter. The role of this parameter is discussed more fully in the Appendix. In Sec. VI the expansion is formulated more precisely in terms of *renormalized propagators*. This leads to a remakable *mass operator variational principle*, the consequences of which are examined in Sec. VII. In Sec. VIII this expansion is compared with some other formal theories, including the Green's-function theory of nuclear matter. Section IX contains a summary of these results. Sections VI, VII, and VIII deal mainly with formal questions, and are not essential for the remainder of the paper.

II. INTERACTION ON AND OFF THE ENERGY SHELL

The most important new idea in Bethe's three-body cluster treatment is the philosophy that when several particles have been excited out of the Fermi sea, they should be allowed to interact with each other *in all possible ways* before dropping back into the Fermi sea. For two excited particles this prescription leads immediately to the usual G matrix. It is also fairly straightforward for three particles, except that one must now be careful to identify and subtract out some spurious first- and second-order terms. With three particles, however, one encounters a new feature. Except for the "first" and "last" G matrices of the generalized ladders in Bethe's summation, all of the G-matrix interactions take place "off the energy shell." In other words, the energy denominators within these G's must include the excitation energy of the third, or "spectator," particle. This is illustrated in Fig. 1(a), where the off-energy-shell denominator e_3 is shown explicitly. For more than three particles, the middle rungs of the generalized ladders will be even further off the energy shell.

On the other hand, it is well known that in the "hole-bubble" diagram, which is superficially very similar to Fig. 1(a), the middle G matrix should be evaluated "on the energy shell." This amounts to a partial summation of Goldstone diagrams, as Bethe, Brandow, and Petschek (BBP)[15] have shown in detail. The nature of this partial summation is indicated in

[15] H. A. Bethe, B. H. Brandow, and A. G. Petschek, Phys. Rev. **129**, 225 (1963). This paper will be referred to as BBP.

Fig. 1(b). The idea is to generalize the relative "time" ordering between the interactions in the "insertion" and "skeleton" parts of the diagram, subject to only one restriction. The relative position of *one* of the v interactions in the insertion must be held fixed. In almost all cases, this fixed or "time-boundary" interaction must be chosen as the *upper* one of the two v interactions by which the insertion is connected to its *external* lines. (In this form, the rule applies to all of the insertions which we shall consider in Sec. IV. A slight modification of this rule will be mentioned in Sec. VI.) This "time boundary" is indicated in Fig. 1(b) by a horizontal bar.

The on-energy-shell result follows from the "factorization theorem,"[16] which is simply an algebraic identity for the products of the energy denominators. The proof of BBP was based on multiple-time integrals of the type used by Goldstone.[17] Similar factorizations can be carried out by means of the multiple-temperature integrals of quantum statistical mechanics, and also by means of Hugenholtz's convolution integrals.[18] A purely algebraic proof of the basic identity has been given by Frantz and Mills.[16] The possibility of applying this idea to the theory of nuclear matter was first suggested by Brueckner and Goldman.[19]

These considerations are vitally important for quantitative calculations. When off-energy-shell propagation is handled correctly,[15] the repulsive effect of the hard core is so strongly enhanced that the Goldstone diagrams for the three-body clusters form a diverging series.[7,20] Therefore it is necessary, and not merely a refinement, to evaluate this series in closed form. Bethe's calculations revealed that previous treatments of three-body effects (which were only valid to third order in G) had led to errors of order 10 MeV per particle for the nuclear matter binding energy.

The "hole-bubble" insertion of Fig. 1(b) is well known to be strongly attractive. Without the g.t.o. (generalized-time-ordering) factorization, however, this insertion would tend to be very far off the energy shell. It would therefore be strongly repulsive. Evidently, the extra Goldstone diagrams which are included in the g.t.o. treatment are also very important quantitatively. The g.t.o. result is also much more convenient. The insertion now depends only on the hole label m, so its interpretation as a self-energy effect is now unambiguous.

We conclude from this discussion that if any further reordering of the Goldstone series is to be done for systems with a strongly repulsive core, it will be essential to pay careful attention to the on or off-energy-shell features of the individual diagrams.

[16] L. M. Frantz and R. L. Mills, Nucl. Phys. **15**, 16 (1960).
[17] J. Goldstone, Proc. Roy. Soc. (London) **A239**, 267 (1957).
[18] N. M. Hugenholtz, Physica **23**, 381 (1957).
[19] K. A. Brueckner and D. T. Goldman, Phys. Rev. **117**, 207 (1960).
[20] This divergence had already been suggested by R. Rajaraman, Phys. Rev. **131**, 1244 (1963).

III. COMPACT CLUSTERS

The considerations of Sec. II suggest the following program: When a diagram can be factorized into two or more parts which are on the energy shell with respect to each other, we shall say that these parts belong to different "compact parts." But where this factorization does not apply to some interaction, as in Fig. 1(a), we shall say that this interaction belongs to the same compact part as the "spectator particles" which are responsible for the off-energy-shell effect. The object is then to perform partial summations of all the Goldstone diagrams which have the same general structure in terms of compact parts. In the final result, the various compact parts must all be on the energy shell with respect to each other.

To make these ideas more precise, we introduce the concept of an *irreducible compact part* (i.c.p.). An n-body i.c.p. is the sum of all Goldstone diagrams, or parts of diagrams, in which n lines enter at the bottom and then proceed to interact in all possible ways, subject to two restrictions: (i) The intermediate states (internal single-particle lines) must all be outside the Fermi sea. (ii) Each of these Goldstone diagrams (or subdiagrams) must include at least one G-matrix element whose energy denominators contain the excitation energies of all n particles. In other words, there must be intermediate states somewhere (perhaps only within a single one of the G matrices) in which all n particles are excited.

For $n=2$ and $n=3$ the i.c.p.'s are just the usual G matrix and Bethe's three-body cluster. In the latter case it is apparent, especially in the higher orders, that the Goldstone diagrams all have a very compact topological structure. Their sum is also compact in coordinate space, in the sense that the correlations are of very short range, hence the name "compact cluster."

The new diagrams are not all "irreducibly compact." In general, each of the new diagrams will consist of several irreducible compact parts. Several examples are shown in Fig. 2 to illustrate the analysis of some typical Goldstone diagrams. Each rectangle indicates an i.c.p.

Note that the topology of the third diagram in Fig. 2 has allowed the hole-scattering interaction to be factorized, permitting this G matrix to become an i.c.p. all by itself. (In cases where there can be no confusion, it is generally more convenient to represent the two-body i.c.p.'s by the usual wiggly-line convention for G.) Factorizations similar to this third example can be carried out whenever all of the lines entering the bottoms of two or more i.c.p.'s are "hole" lines. The same is true whenever all the lines leaving the tops of two or more i.c.p.'s are hole lines.

The last example in Fig. 2 demonstrates that the diagram analysis, as stated so far, is sometimes ambiguous. The middle G matrix could be associated with either the upper or the lower of the two i.c.p.'s. This

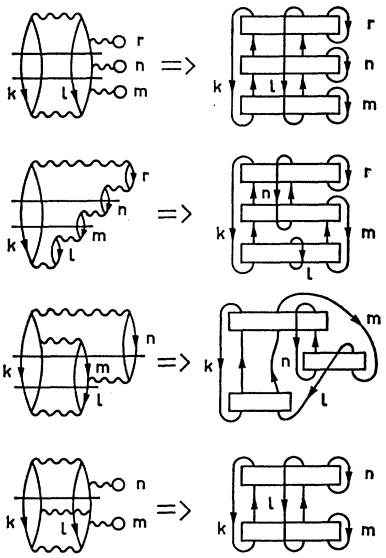

FIG. 2. Analysis of some typical Goldstone diagrams into their irreducible compact parts.

ambiguity can arise whenever two i.c.p.'s are connected together by two or more upgoing or "particle" lines. The ambiguity disappears if one adapts the convention that all interactions among these "connecting particle lines" must be associated with the *lower* of the two i.c.p.'s. The *upper* i.c.p. must begin with an interaction involving some particle other than those in the connecting lines. (The words *upper* and *lower* could just as well be interchanged here, as long as the rule is followed consistently.)

This is as far as we have carried the analysis of the most general compact-cluster diagram. The details of any particular diagram can be deduced from the rules for the Goldstone expansion. The foregoing discussion will suffice for the purposes of this paper.

At this point we should comment on the similarity to the expansion of Lee and Yang for quantum statistical mechanics.[21,22] Our n-body i.c.p.'s correspond to their n-body generalized ladders, or multiple collision operators. There is an important difference, however. In their expansion, the exclusion effect of the almost-fully-occupied Fermi sea is not taken into account consistently from the beginning. The intermediate-state particle lines which connect up the various generalized ladders carry statistical weighting factors (corresponding to the usual exclusion operator and to the true occupation probabilities discussed here in Sec. VI), but this is *not* true of the intermediate states within their ladders. Diagrams corresponding to the exclusion effect *within* their ladders can, however, be identified among the higher order terms of their expansion.[23] It seems likely that the present expansion could be obtained by suitable rearrangements of their expansion. Also, their diagram rules might be helpful if one should wish to express the rules for the new series directly in terms of the i.c.p.'s.

Mohling has used the Lee-Yang expansion as the starting point for his theory of nuclear matter.[24] However, he has expanded the multiple-collision operators in terms of two-body reaction matrices, which is just what we are now trying to avoid. Other features of Mohling's theory are discussed in Refs. 25 and 26.

IV. SINGLE-PARTICLE POTENTIALS

The importance of summing out the self-energy insertions by introducing single-particle potentials is quite familiar in nuclear matter theory. The present scheme restricts our choice of self-energy insertions to just those ones which can be placed *entirely* on the energy shell by the g.t.o. factorization. Fortunately, these insertions are very easy to identify. All one need do is to examine their *external* lines, by means of which they are connected to the skeleton. The on-energy-shell insertions are just those for which the external lines cross over each other. The reason for this should be clear from our discussion of Fig. 1(b).

The sum of all these allowed insertions defines an "on-energy-shell mass operator" M^{on}. Similarly, one can say that the sum of all the self-energy-like parts which do *not* satisfy this crossed-line rule will define an "off-energy-shell mass operator" M^{off}. (In a later paper we shall attribute the bulk of the rearrangement energy to M^{off}.) The simple external-line rule breaks down in cases where the external lines are joined directly to each other by a single v interaction. Since this v is the first term of a Brueckner ladder, we assign these insertions to M^{on} in the case of normally occupied or "hole" states, and to M^{off} for the intermediate or "particle" states. The contributions to M^{on} can all be expressed in terms of irreducible compact parts, as described in the previous section.

We shall now describe the first few terms in $U(b)$ and $U(m)$. We follow the notation of BBP, where intermediate states are denoted by a, b, c, etc., and normally occupied states are labelled l, m, n, etc.

Intermediate-State Potentials

The intermediate-state insertions are easily disposed of. They all have the general form shown in Fig. 3(a). This structure suggests a simple physical interpretation for $U(b)$. Since the intermediate state b is now occupied, as part of the "skeleton" cluster, the exclusion principle must prevent "other" particles from scattering into

[21] T. D. Lee and C. N. Yang, Phys. Rev. **113**, 1165 (1959); **117**, 22 (1960).

[22] C. Bloch, in *Studies in Statistical Mechanics*, edited by J. de Boer and G. E. Uhlenbeck (North-Holland Publishing Company, Amsterdam, 1965), Vol. III.

[23] I am grateful to Dr. A. G. Petschek for explaining this to me. See also Refs. 22 and 25.

[24] F. Mohling, Phys. Rev. **122**, 1043 (1961); **122**, 1062 (1961); **124**, 583 (1961); and **128**, 1365 (1962).

[25] A. G. Petschek, Ann. Rev. Nucl. Sci. **14**, 29 (1964).

[26] J. S. Bell, in *Proceedings of the Rutherford Jubilee International Conference, Manchester, 1961* (Academic Press Inc., New York, 1961), p. 373.

this state. This blocking effect decreases the phase space available to all the "other" clusters, so this must decrease the total binding energy. According to Eq. (4.1), below, this must correspond to a *positive* $U(b)$.

The leading term is shown in Fig. 3(b). We have estimated this to be about +1.5 MeV for $k_b=k_F$, decreasing to around +.75 MeV at $k_b=\pi/2c=2.6k_F$, the latter being a typical value for the momenta of the intermediate states admixed by a hard core of radius c. [See Eq. (7.17) of BBP. At present we are assuming $k_F=1.36$ F^{-1} and $c=0.45$ F. These estimates for $U(b)$ were obtained by scaling from Fig. 14 of BBP. One should note that the units in this figure are based on the Brueckner-Gammel-Thaler value of c, namely 0.40 F.] Assuming +1 MeV for the average value of $U(b)$, one can see from Eq. (4.1) that this contributes only around +0.1 MeV to the total E/N. This shows that $U(b)$ is quite negligible for nuclear matter. One should, however, expect this to be relatively larger and more significant for liquid He^3.

The reason why $U(b)$ is so small is that when particles are excited out of the Fermi sea, they are usually thrown very far out by the hard core. The probability that two clusters will be competing for the same state b is therefore very small.

The occupation probabilities of the intermediate states are typically only of order 0.15%. This can be seen as follows. Typical values for the momenta of states inside and outside of the Fermi sea are $(\sqrt{0.6})k_F$ and 2.6 k_F, respectively. The probability of a state in the Fermi sea being empty is around 0.12 [see Eq. (4.2) below]; therefore, the probability of an intermediate state being filled should be of order $0.12\times[(\sqrt{0.6})/2.6]^3=0.3\%$. This is actually an overestimate, because of the long "tail" in the momentum distribution caused by a hard core. This can be seen in Fig. 14 of BBP.

Occupied-State Potentials

The potentials $U(m)$ for the normally occupied states are much larger and more interesting. The leading terms are shown in Fig. 4. The first term is the usual "hole-bubble" insertion. This term has been extensively discussed in the literature. Following Ref. 1 we shall call this the "two-body Hartree-Fock potential" $U_2(m)$. By analogy, we shall call the next term the "three-body Hartree-Fock potential" $U_3(m)$. For an "average particle" in the Fermi sea, this term is *three times* as large as Bethe's three-body cluster energy E_3/N, for the same reason that $\langle U_2(m)\rangle_{\rm av}$ is twice the two-body cluster energy E_2/N.

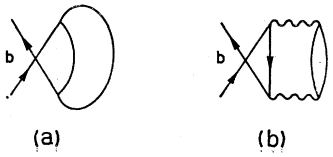

FIG. 3. Self-energy insertions for the intermediate states. All have the general form (a). The leading term is (b).

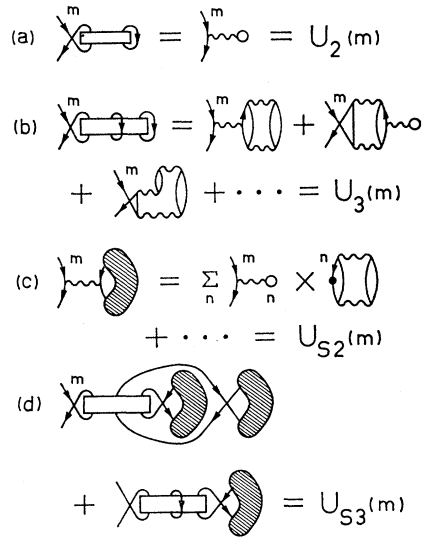

FIG. 4. The leading terms for the potential of an occupied state m: (a) the two-body Hartree-Fock potential U_2, (b) the three-body Hartree-Fock potential U_3, (c) the two-body saturation potential U_{S2}, and (d) the three-body saturation potential U_{S3}.

Three-Body Cluster Energy

It will be helpful to have some numerical estimates for the various terms in E/N and $U(m)$. We shall now estimate E_3/N, the three-body compact-cluster energy, by following Bethe's argument.[7] He has shown that this can be calculated as if it were a self-energy correction to E_2/N. [It would be wrong, of course, to say that the three-body clusters are *simply* a self-energy correction to the two-body clusters. We have already argued that E_2/N and E_3/N should be calculated separately. This self-energy argument should simply be viewed as a convenient way to estimate E_3/N. It does not imply any change in the calculation of E_2/N, which should be carried out with $U(b)\approx 0$, as discussed above.]

According to the G-matrix perturbation theory of Moszkowski and Scott[27] and BBP, the *change* in the two-body interaction energy which results from a moderate change in the single-particle potentials is simply

$$\delta(E_2/N)=\kappa[\langle\delta U(b)\rangle_{\rm av}-\langle\delta U(m)\rangle_{\rm av}]. \qquad (4.1)$$

The dimensionless coefficient is

$$\kappa=\rho\int|\zeta(\mathbf{r})|^2 d\tau. \qquad (4.2)$$

Here ρ is the ordinary nuclear density, and $\zeta=\phi-\psi_{\rm BG}$ is the "wound" in the correlated two-body (Bethe-Goldstone) wave function, calculated for an "average pair" in the Fermi sea. For the sake of illustration, we shall assume that $\kappa=0.12$ at the normal nuclear matter density. [This value of κ is based on preliminary results

[27] S. A. Moszkowski and B. L. Scott, Ann. Phys. (N. Y.) **11**, 65 (1960).

of calculations by Dahll and Østgaard.[28] The normal nuclear matter density is taken to be[29,30] $k_F=1.36$ F^{-1}, $\rho=0.17$ F^{-3}.] The $\delta U(b)$'s in (4.1) should be averaged with respect to $|\langle \mathbf{k}_b|\zeta\rangle|^2$, the square of the Fourier transform of ζ (Fig. 14, BBP), whereas a simple average over the states in the Fermi sea will generally suffice for $\delta U(m)$.

Bethe's prescription for the appropriate $\langle \delta U(b)\rangle_{\rm av}$ is roughly the following. One should first calculate $U(b)$ the old way, as described in BBP. The hard-core contribution to this $U(b)$ should then be reduced by a factor of 3 to take account of all the higher order Goldstone diagrams within the compact three-body cluster. According to line 5 of Table II of Bethe's paper, the appropriate value of $\langle \delta U(b)\rangle_{\rm av}$ is around -30 MeV. This is to be multiplied by $\kappa=0.12$. We shall then subtract off $\frac{1}{3}$ of this result, to account in a rough way for the reduced effectiveness of the tensor force in the more complicated three-body geometry. [About $\frac{1}{3}$ of our estimate for κ is due to the tensor-induced $^3D_1$ wave. See Fig. 13 of BBP and also Fig. 2(a) of Brueckner and Masterson.[31]] Our final result is $E_3/N\approx -2.4$ MeV. (This is larger than Bethe's result, mainly because we assume a larger value for the parameter κ.) From this we obtain $\langle U_3(m)\rangle_{\rm av}=3\ E_3/N\approx -7.2$ MeV. These figures are obviously very rough. Still, they demonstrate that the three-body terms are quite significant, and that they really deserve a careful treatment.

Two-Body Cluster Energy

We can now estimate E_2/N. Following Weisskopf,[32] we *assume* that the theory and the bare two-body interaction are both correct, in the sense that they should give the correct results. We then neglect all the higher order contributions, so that

$$E/N=\tfrac{3}{5}T_F+E_2/N+E_3/N. \tag{4.3}$$

Inserting $E/N=-16$ MeV, $\frac{3}{5}T_F=+23$ MeV, and $E_3/N=-2.4$ MeV, we find that $E_2/N\approx -36.6$ MeV. It follows that

$$\langle U_2(m)\rangle_{\rm av}=2E_2/N\approx -73 \text{ MeV}.$$

True Occupation Probabilities, Saturation Potentials

The third term shown in Fig. 4 is also quite significant. This represents a renormalization of $U_2(m)$ due to the fact that the normally occupied states n are actually occupied less than 100% of the time. This interpretation was first proposed by Thouless.[33] The closed-diagram part on the right-hand side of Fig. 4(c) is the first nontrivial term in Thouless' expansion[34] for the *true* single-particle occupation probability

$$P_n=\langle \Psi_g|\, a_n^\dagger a_n\,|\Psi_g\rangle. \tag{4.4}$$

Here Ψ_g is the *true* wave function for the N-body ground state, normalized to unity. (For the normally occupied states, the first term in Thouless' expansion is just unity.) For an "average state" n [$k_n\approx(\sqrt{0.6})k_F$], the contribution to $1-P_n$ from this diagram part is just the κ of (4.2). We shall assume, for the sake of illustration, that $\langle 1-P_n\rangle_{\rm av}=\kappa=0.12$. The contribution from Fig. 4(c) is

$$U_{S2}(m)=\langle P_n-1\rangle_{\rm av}U_2(m), \tag{4.5}$$

and its average value is therefore $\langle U_{S2}(m)\rangle_{\rm av}=\langle P_n-1\rangle_{\rm av}\langle U_2(m)\rangle_{\rm av}\approx(-0.12)\times(-73 \text{ MeV})=+8.8$ MeV. We have argued elsewhere that this term plays an important role in determining the saturation properties of actual nuclei.[5] For this reason we call it the "two-body saturation potential" U_{S2}.

The last term in $U(m)$ which we shall consider is the "three-body saturation potential"

$$U_{S3}(m)=[\langle P_nP_{n'}\rangle_{\rm av}-1]U_3(m). \tag{4.6}$$

This is shown in Fig. 4(d). It is quite analogous to U_{S2}, in the sense that it represents a corresponding renormalization of U_3. Replacing P_n by $1-\kappa$, we find that $\langle P_nP_{n'}\rangle_{\rm av}-1\approx\kappa^2-2\kappa$, hence $\langle U_{S3}(m)\rangle_{\rm av}\approx+1.6$ MeV, which is not quite negligible. In particular, this term has a very strong density dependence, and for this reason we think it may be significant for finite systems.

One should note that the saturation terms $U_{S2}+U_{S3}$ together constitute around -15% of the *total* $U(m)$. This is large enough so that one should consider corrections to the simple assumption $\langle P_n\rangle_{\rm av}=1-\kappa$. A consistent treatment of *all* the higher order contributions coming from two-body correlations is described in LCE.[13] [See also Eqs. (6.3), (6.4) below.] The decrease of P_n due to the three-body correlations should also be examined, as well as the differences between the individual P_n's and their average value.

Since the quantities $P_n<1$ occur here in a natural way, one should expect to find similar terms associated with the intermediate or "particle" states. This is indeed true, as shown in Sec. VI. The effect of these terms is to multiply each particle line by a weighting factor of $(1-P_b)$. *In practice*, however, their effect is not worth considering for two reasons: (i) The P_b's are very small to begin with. We have argued at the beginning of this

[28] G. Dahll and E. Østgaard (private communication). These investigators are making a detailed study of the two-body correlations, including tests of various approximation methods for G, $\langle \mathbf{k}|\zeta\rangle$, and κ. The calculations are based on a hard-core potential, instead of a soft core, simply as a matter of convenience. The above estimate assumes that $\frac{1}{3}$ of κ arises from the large $^3D_1$ wave induced by the tensor force. Recent results indicate that the $^3D_1$ contribution is considerably larger than this, and that κ may be as large as 0.16.

[29] L. R. B. Elton, *Nuclear Sizes* (Oxford University Press, London, 1961).

[30] B. H. Brandow (to be published).

[31] K. A. Brueckner and K. S. Masterson, Jr., Phys. Rev. 128, 2267 (1962).

[32] V. Weisskopf, Nucl. Phys. 3, 423 (1957).

[33] D. J. Thouless, Phys. Rev. 112, 906 (1959).

[34] D. J. Thouless, *The Quantum Mechanics of Many-Body Systems* (Academic Press Inc., New York, 1961), p. 47. For an alternative derivation, see A. E. Glassgold, W. Heckrotte, and K. M. Watson, Phys. Rev. 115, 1374 (1959).

section that their order of magnitude is only 0.15%; (ii) If these terms are treated as perturbations, it is easily seen that there are no terms in the total energy which are linear in P_b. Their effect first appears in terms of order $P_bP_{b'}$. The argument is completely analogous to the discussion in Sec. VI of the energy corrections arising from $P_n<1$.

V. PHYSICAL MOTIVATIONS AND CONSEQUENCES

The particular choices of rearrangements or partial summations made in Secs. III and IV are based on two assumptions: (1) that the normally occupied states are nearly always occupied, and similarly that the intermediate states are nearly always empty, and (2) that the most important correlations are between particles deep within the Fermi sea. These assumptions are well justified for nuclear matter, and presumably also for liquid He^3.

The correlations between particles deep in the Fermi sea *must* heal rapidly. This is due primarily to exclusion, as Gomez, Walecka, and Weisskopf[35] have emphasized, but the reference-spectrum method[15] has demonstrated that the single-particle potential energies and the off-energy-shell effects also contribute in an important way. For all of these reasons, the correlations within the compact-cluster diagrams *must* be of quite short range.

It follows directly from this rapid healing property that the order of magnitude of a general compact-cluster diagram is proportional to $\kappa^{h'-1}$, where κ is the quantity introduced in (4.2). Here h' is the number of *independent* hole-line summations. (Note that momentum conservation can sometimes restrict the hole-line summations.) This means that the Brueckner-Bethe-Goldstone theory has finally been cast into a form which has an obvious small parameter. A general argument for this $\kappa^{h'-1}$ proportionality is given here in the Appendix.

That κ should be the natural expansion parameter is not hard to guess. Essentially the same parameter can be found in the Jastrow cluster expansion.[36]

According to (4.2), κ is just the density multiplied by the volume of the "wound" ζ. This volume can be regarded as a more precise definition of the "healing distance" introduced by Gomez *et al.* The connection is

$$\int |\zeta(\mathbf{r})|^2 d\tau \equiv \tfrac{3}{4}\times\frac{4\pi}{3}\lambda^3. \tag{5.1}$$

(We include a factor of $\frac{3}{4}$ for the probability that two particles can interact in a relative S state, since $|\zeta|^2$ refers here to an "average pair".) For $\kappa=0.12$ and $\rho=0.17$ F^{-3}, this λ turns out to be 0.61 F. One should note that this is considerably smaller than the "separation distance" of Moszkowski and Scott,[27] which can also be considered a healing distance. The present definition is more relevant for questions of convergence.

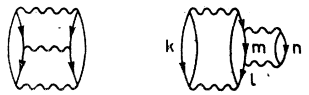

FIG. 5. Correction terms due to scattering within the Fermi sea.

Gomez *et al.* proposed that the convergence of nuclear matter theory could be understood from the fact that the healing distance is considerably smaller than the average particle spacing. We see that κ is just $(\frac{3}{4})(\lambda/r_0)$,[3] where $r_0=(4\pi\rho/3)^{-1/3}=1.12$ F.[29,30] This observation has been used for many years as a plausibility argument for various forms of "independent-pair" approximations. Bethe's work was the first to show how this essentially geometric quantity emerges from the perturbation formalism.

Another important feature is that κ contains a factor of ρ; thus we are expanding in powers of the density. Hugenholtz observed long ago[37] that this should be the most natural procedure for a low-density system. One should note, however, that this is *not* a simple Taylor expansion in ρ. We are only using ρ to order the terms according to their general orders of magnitude. The *detailed* ρ dependence of each term remains rather complicated. Indeed, it would not be sensible to use a straight Taylor expansion in ρ for a bound, saturating system, since at low densities the system becomes unstable against condensation into "droplets." (This objection does not apply to an unbound system such as a hard-sphere gas.)

We now consider two examples to illustrate some further aspects of the expansion. All three of the G matrices in Fig. 5(a) are on the energy shell, and each is therefore an i.c.p. This diagram results from the unsymmetrical treatment of the "particle" and "hole" states. "Upgoing" ladders are summed out immediately, as required by the hard core, whereas the "downgoing" ladders, of which Fig. 5(a) is the simplest example, are treated as perturbations. A number of people have observed that the downgoing ladders can be included along with the upgoing ones by a suitable redefinition of G.[38] The reason for rejecting this proposal is that this

[35] L. C. Gomez, J. D. Walecka, and V. F. Weisskopf, Ann. Phys. (N. Y.) **3**, 241 (1958).

[36] See, for example, S. Drell and K. Huang, Phys. Rev. **91**, 1527 (1953); R. Jastrow, *ibid.* **98**, 1479 (1955); K. A. Brueckner, C. A. Levinson, and H. M. Mahmoud, *ibid.* **95**, 217 (1954) (Appendix); J. S. Bell and E. J. Squires, Phil. Mag. Suppl. **10**, 211 (1961); J. W. Clark and P. Westhaus, Phys. Rev. **141**, 833 (1966). This last paper contains an extensive review of the literature, as well as a thorough discussion of the higher order terms.

[37] N. M. Hugenholtz, Physica **23**, 533 (1957).

[38] B. M. Galitski, Zh. Eksperim. i Teor. Fiz. **34**, 151 (1958) [English transl.: Soviet Phys.—JETP **7**, 104 (1958)]; F. Iwamoto, Progr. Theoret. Phys. (Kyoto) **22**, 903 (1959); **23**, 871 (1960); J. S. R. Chisholm and E. J. Squires, Nucl. Phys. **13**, 156 (1959); M. L. Mehta, *ibid.* **12**, 333 (1959); S. A. Moszkowski and A. M. Sessler, *ibid.* **18**, 669 (1960); D. J. Thouless, Ann. Phys. (N. Y.) **10**, 553 (1960); R. E. Prange, in *Lectures on Field Theory and the Many-Body Program*, edited by E. R. Caianiello (Academic Press Inc., New York, 1962); A. G. Petschek (unpublished); E. L. Lomon and M. McMillan, Ann. Phys. (N. Y.) **23**, 439 (1963).

would destroy the very useful "healing" property of the correlations, and thereby ruin the rapid convergence of the higher order terms. Their G matrix is also more difficult to compute accurately.

The effect of the hole-hole scatterings is so small that they may quite properly be regarded as perturbations. Following the discussion of Rajaraman,[39] we estimate that the contribution of Fig. 5(a) is only of order -0.25 MeV. This is less than 1% of E_2/N. Rajaraman has shown that this term is especially small because the requirements of momentum and spin conservation both very strongly reduce the phase space for the hole-line summations.

Figure 5(b) represents the scattering of particle m *into* state l during the time particle l is elsewhere. This is also only a small perturbation, because the hole in state l is only virtual.[40] All four of the G matrices are on the energy shell (and are therefore i.c.p.'s), but the *middle* energy denominator is very large. We estimate that the E/N contribution from this term is only of order -0.2 MeV.

These two diagrams represent the simplest corrections to the initial assumption that no intermediate states are available within the Fermi sea. The perturbations are extremely small, which demonstrates that this assumption is an excellent starting point for the expansion. As with all the other terms in the compact-cluster series, the higher order analogues of these processes must decrease rapidly with increasing numbers of independent hole-line summations. On the other hand, the number of distinct diagrams increases very rapidly with the number of hole lines, since these terms are not "compressed" into i.c.p.'s the way the repeated particle-interaction ladders are. For this reason it appears very likely that we are dealing with an asymptotic expansion.[41] But this should not detract from the practical utility of the expansion, since the point at which the series might begin to diverge should be very far beyond any number of terms that one could compute in practice.

Long-Range Correlations and Degeneracy

The rapid decrease in the magnitudes of the first few terms of our expansion is certainly physically meaningful, because the binding energy is clearly dominated by the short-range few-body correlations. On the other hand, one knows that there are long-range correlations among the particles near the Fermi surface. These are important for phenomena such as pairing and collective oscillations.

These long-range effects are artificially suppressed by the large energy denominators. Note that the occupied-state potentials are strongly attractive, while the intermediate-state potentials are all weakly repulsive. This places a lower bound of quite large magnitude (>100 MeV) on *all* of the energy denominators. This means that the long-range effects are relegated to the terms of very high order. In a formal sense these effects are still contained in the expansion, but they are quite inaccessible for practical purposes.

Consider the famous example of the BCS correlations. These correspond to a very strong mixing, or near degeneracy, of the low-lying configurations.[42] This invalidates the nondegenerate assumption upon which the Goldstone expansion and the present one are based. This means that there must almost certainly be a divergence somewhere in the formalism. In some previous formulations of nuclear matter theory, the BCS phenomenon could produce a divergence already in the leading term consisting of a single G matrix. In the present case this must take the form of an asymptotic divergence. This latter form of divergence is much less offensive. Of course it would be nice to eliminate this divergence and to be able to study the BCS correlations in detail. This can be done by an extension of the present scheme. (It may well be, however, that the resulting expansion is still asymptotically divergent for other reasons, as mentioned above.)

Long-range correlations between particles near the Fermi surface can generally be thought of in terms of a strong configuration mixing of the low-lying unperturbed eigenstates (N-body Slater determinants). This problem can be handled by employing the present types of partial summations in the context of the *degenerate* linked-cluster expansions.[9–13]

These degenerate expansions have a very useful feature. They permit a clean separation (at least in principle) between the problem of the short-range correlations, which form the main subject of nuclear-matter theory, and the long-range correlations which are studied in Fermi liquid theory and in the shell model. The "closed-shell" part of the problem is treated exactly as in the Goldstone expansion, whereas the "valence particles" near the Fermi surface are treated by means of a "reduced Hamiltonian." The latter is quite analogous to the semiphenomenological Hamiltonians introduced by Bardeen, Cooper, and Schreiffer,[43] and by Landau.[14] For finite nuclei this can be identified with the usual shell-model Hamiltonian. The result is convenient and not at all surprising. But it is nice that this can be formulated precisely.

This clean separation of the many-body problem was accomplished by Bloch and Horowitz.[9,10] However, their treatment of the degenerate or valence part of the system was subject to unlinked-cluster difficulties.

[39] R. Rajaraman, Phys. Rev. **129**, 265 (1963).

[40] This diagram has been discussed previously by K. A. Brueckner and D. T. Goldman, Phys. Rev. **117**, 207 (1960), and by K. A. Brueckner, J. L. Gammel, and J. T. Kubis, *ibid.* **118**, 1438 (1960).

[41] Other aspects of the asymptotic nature of the Goldstone expansion have been discussed by A. Katz, Nucl. Phys. **20**, 663 (1960) and *The Many-Body Problem*, edited by C. Fronsdal (W. A. Benjamin and Company, New York, 1962), and by G. A. Baker, Phys. Rev. **131**, 1869 (1963).

[42] N. N. Bogolubov, Physica **26**, S1 (1960).

[43] J. Bardeen, L. N. Cooper, and J. R. Schrieffer, Phys. Rev. **108**, 1175 (1957).

This restricted applications of their formalism to nuclei with only a few valence particles. We have removed this limitation by deriving a completely linked version of their expansion[12,13] following a previous attempt by Morita.[11]

In applying this formalism, the first step is to derive and calculate the appropriate reduced Hamiltonian. The partial summations of this paper should be useful here. The second step is to solve the resulting secular equation. In most cases this can only be done approximately. The BCS and random-phase techniques may be introduced at this stage. Another possibility is to treat the reduced Hamiltonian by a *second* application of linked-cluster perturbation methods. In such an approach one must be careful not to confuse the new diagrams with the "compact-cluster" diagrams used in the first step. The old and new diagrams span different configuration spaces.

By analogy with the Fermi liquid theory, one can say that the reduced Hamiltonian describes the system's "quasiparticle" degrees of freedom. This is one way of giving a precise meaning to the notion of a Landau quasiparticle. The new diagrams just mentioned are therefore "quasiparticle diagrams." Further discussion of the degenerate formalism will be reserved for a later paper.

VI. FORMULATION IN TERMS OF RENORMALIZED PROPAGATORS

The full consequences of introducing the on-energy-shell mass operator M^{on} can most conveniently be expressed in terms of renormalized propagators. To avoid possible confusion, we wish to emphasize that the term "propagator" will be used here simply to mean a class of partial summations. These summations can all be carried out by pure algebraic, time-independent methods. There are many points in common between a Green's function and this concept of a propagator, but it is important to realize that they differ in detail. In particular, we do *not* use the *causal* Green's function. We shall introduce the propagator concept by easy stages.

Let us return to Fig. 1(b). This consists of two self-energy parts connected by two "propagator" line segments. We have tacitly assumed that the left-hand part is the "skeleton," the right-hand part representing a self-energy insertion into this skeleton. This assumption can be generalized as follows. Consider all the propagator line segments belonging to a particular "self-energy cycle." For a translationally invariant system these propagator segments will all carry the same label, and, together with the "skeleton" and "insertion" parts, they will form a closed loop. Examples are shown in Fig. 6. If one now examines the relative "times" of the *upper* ends of all the propagator segments, one of them will, of course, be the highest. It is very tempting to say that the skeleton is that part which is attached to the highest point contained in the set of all the propagator line segments.

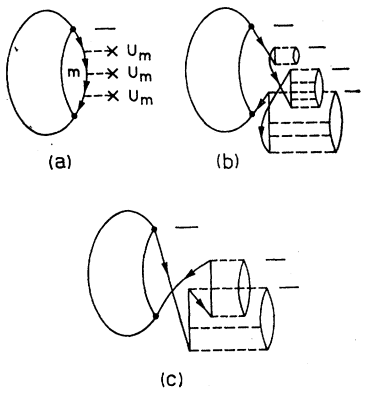

FIG. 6. Diagrams corresponding to the expansion of Eq. (6.1).

Self-Energy Propagator

Suppose, for the moment, that we adopt this convention. Now take a given skeleton part and add all possible self-energy insertions to its propagator line, including each insertion an arbitrary number of times. In accordance with the above convention, the time boundaries of these insertions must all be placed *below* the time boundary of the skeleton. The relative time ordering of the insertions can be quite arbitrary in other respects. After applying the g.t.o. factorization, the result will simply be to replace the "unperturbed propagator energy" $E_m{}^0$ by the "full propagator energy" $E_m{}^0+U_m$ in the denominators at all the levels where this line m appears in the skeleton. The potential U_m [previously written $U(m)$] is determined by the equation

$$U_m=M_m{}^{\text{on}}(E^0{}_m+U_m). \tag{6.1}$$

The diagrams for the on-energy-shell mass operator $M^{\text{on}}(\omega)$ are evaluated according to the usual rules,[44] with the following modifications. First, *erase* the external lines. The overall sign factor is $(-1)^{l+h}$, where l and h are now the numbers of *internal* closed loops and hole-line segments. Secondly, *close* the diagram by adding a single line to replace the pair of external lines. In determining the energy denominators this line carries an "unknown" energy ω. These rules apply to the $M_b(\omega)$ for intermediate states, as well as for $M_m(\omega)$.

One should note that in (6.1) we have written $E_m{}^0$ for the unperturbed energy instead of just the kinetic energy T_m. This is to emphasize that very similar results are obtained when one starts with a "counter term" in the unperturbed Hamiltonian $H_0=T+U^0$, $V=v-U^0$. The final U_m emerging from (6.1) is then the *difference* between what one would obtain for $E_m{}^0=T_m$ and the "unperturbed" potential $U_m{}^0$. In any event, the *total* potential $U_m+U_m{}^0$ should be independent of the starting point $U_m{}^0$. It is especially

[44] A concise and unambiguous statement of the diagram rules is given in LCE.

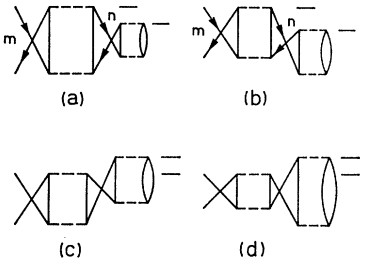

FIG. 7 Diagrams summed by the complete propagator for state n.

useful to allow for this generalization in the finite case, as will be discussed in a later paper. There we will want to choose the $U^0{}_m$'s, which will constitute the "shell-model potential," such that the "corrections" arising from (6.1) will turn out to be zero.

The structure of the diagrammatic expansion which corresponds to (6.1) can most easily be understood by working backwards from the result. Let us expand the potential U_m out of the denominators of the skeleton, as illustrated in Fig. 6(a), and then replace each "potential interaction" by a mass-operator diagram. Following the discussion of Fig. 1(b), the time boundary of each insertion must be fixed at the level of the U_m interaction which it represents. The g.t.o. factorization can then be reversed to convert each on-energy-shell insertion into a sum of Goldstone diagrams with various relative time orders. This last step is illustrated in Fig. 6(b). Note that this leads to a string of insertions whose time-boundaries occur in the "natural order" shown in Fig. 6(a). The complete self-energy expansion also includes many insertions whose time boundaries are *not* in this natural order. A simple example is shown in Fig. 6(c). There the lower time boundary belongs to a "second generation" insertion, corresponding to a self-energy correction to the denominators of the "first-generation" insertions shown in Fig. 6(b). In higher orders there are also "third-generation" insertions which correct the energy denominators of the "second-generation" insertions, and so on. The complete expansion corresponding to (6.1) contains insertions into insertions *ad infinitum*, in other words, "higher-generation" insertions of all orders. This general structure of the propagator expansion has been extensively discussed in LCE (Secs. III and IV). [Des Cloizeaux[45] has discussed the perturbative expansion of (6.1) from a different point of view, in terms of Lagrange's expansion formula. The detailed relation between Lagrange's formula and the diagrammatic expansion is, however, far from transparent.]

The virtue of defining the skeleton as the self-energy part with the highest time boundary is that this would appear, from a naive analysis, to eliminate the overcounting problem in the renormalized expansion of the closed diagrams. This is only an illusion, however. For example, this would not eliminate the overcounting problem discussed below in connection with Fig. 8(f). Worse still, this would overlook an important class of diagrams which can be summed out by a more general definition of the propagators.

[45] J. Des Cloizeaux, Nucl. Phys. **20**, 321 (1960). See also A. Klein, Ref. 47.

Complete Propagator

Consider the four diagrams shown in Fig. 7. The right-hand sides of these diagrams all represent insertions into a self-energy diagram for U_m. Here there is no doubt which side is inserted into the other, since the "skeleton" side is now determined by the external lines. All four of these diagrams are distinct, and therefore it would be nice to choose a renormalization scheme which would automatically include them all. We shall do this by redefining what is meant by the propagator for the state n.

First, we should point out the significance of diagrams 7(c) and 7(d). The factorization theorem shows that their sum is equal to

$$U_m{}^{(2)}\frac{\partial M_n{}^{(2)}(\omega)}{\partial\omega}\bigg|_{\omega=E_n{}^0}. \tag{6.2}$$

This is just the second-order term in U_m multiplied by the lowest order contribution to the quantity P_n-1. It can be shown, from Thouless's expansion for the expectation value of a general one-body operator,[34] that the *true* occupation probability of state n is

$$P_n\equiv\langle\Psi_g|a_n{}^+a_n|\Psi_g\rangle = \left[1-\frac{\partial M_n(\omega)}{\partial\omega}\right]^{-1}\bigg|_{\omega=E_n{}^0+U_n}. \tag{6.3}$$

Here Ψ_g is the true wave function of the interacting ground state. Diagrams 7(c) and 7(d) correspond to the first term of the geometric series

$$(1-M')^{-1}=1+M'+(M')^2+\cdots. \tag{6.4}$$

The *complete renormalized propagator* for state n will now be defined as the partial summation of all repetitions of insertions of the on-energy-shell mass operator, *without any restrictions* on the positions of their time boundaries. The time boundary of the skeleton can now be overlapped, as in diagrams 7(c) and 7(d), by an *arbitrary* number of self-energy parts. These parts correspond to the geometric series (6.4). Other self-energy parts will lie entirely *below* the skeleton time boundary, as in diagrams 7(a) and 7(b), or entirely *above* this. Their effect is simply to replace $E_n{}^0$ by $E_n{}^0+U_n$ in all the energy denominators of the skeleton, and similarly in (6.4).

For those insertions lying *entirely above* the skeleton time boundary, it is necessary to redefine the insertion time boundary as the *lower* one of the two v interactions by which the external lines are connected to the insertion. After this modification, it can easily be seen that the complete propagator is a "faithful" partial sum-

mation, i.e., it includes each possible relative time ordering once and only once.

In addition to the expected self-energy correction, this partial-summation multiplies the downgoing line n by a factor P_n. Note that there is *only one* factor of P_n for the renormalized downgoing line, no matter how many interactions occur in *other parts* of the skeleton during the "time" interval between the ends of this line. We have used this result in the previous section, where the P_n-1 corrections to U_m were called "saturation" terms.

The complete propagator for an intermediate state b is quite similar. The main difference is in the physical interpretation of the weighting factor for the upgoing line. This factor is

$$1-P_b=1-\langle\Psi_g|a_b^\dagger a_b|\Psi_g\rangle=\langle\Psi_g|a_b a_b^\dagger|\Psi_g\rangle$$
$$=\left[1-\frac{\partial M_b(\omega)}{\partial\omega}\right]^{-1}\Bigg|_{\omega=E_b^0+U_b}. \tag{6.5}$$

Overcounting of the Interaction Energy Diagrams

One might naively guess that the original Goldstone series would be reproduced by summing all the irreducible closed diagrams (skeletons with no self-energy insertions) and interpreting each line as a complete propagator. This is quite wrong because this procedure counts many of the higher order Goldstone diagrams two or more times. This can easily be seen from Fig. 7. If we close the line m on itself and then sum the indices m and n over all occupied states, we obtain two distinct Goldstone diagrams which are each counted twice. (This particular problem does not occur when self-energy propagators are used instead of complete propagators.)

A related problem is that the two-body interaction energy of nuclear matter, $E_2/N\approx-36$ MeV, would appear to be reduced by a factor of $\langle P_mP_n\rangle_{\rm av}\approx(1-\kappa)^2\approx0.78$. Quite fortunately, this strong renormalization of E_2/N does not occur. This can easily be seen by introducing U_m into the unperturbed Hamiltonian and subtracting this from the perturbation. The relevant terms in the interaction-energy expansion are shown in Fig. 8. The shaded parts represent the weighting factor corrections (P_m-1), (P_n-1), i.e., they correspond to the entire geometric series in (6.4). Consider the diagram 8(f), which resembles the $U_{S2}(m)$ contribution to 8(c). In factorizing the ends of this diagram, one finds that each of the corresponding Goldstone diagrams is counted twice. The ends become indistinguishable when either one, (P_m-1) or (P_n-1), can contain the highest interaction of the entire diagram, so one must give the factorized diagram a weight of $\frac{1}{2}$. This is quite analogous to the factor of $\frac{1}{2}$ in diagram 8(a). The $U_2(m)$ and $U_3(m)$ terms in diagram 8(c) just cancel off the diagrams 8(d) and 8(e). The $U_{S2}(m)$ term is now twice as large as 8(f), however, so the final expression contains a left-over term equal to *minus* 8(f). This overcounting problem was noted by Brueckner, Gammel, and Kubis.[40]

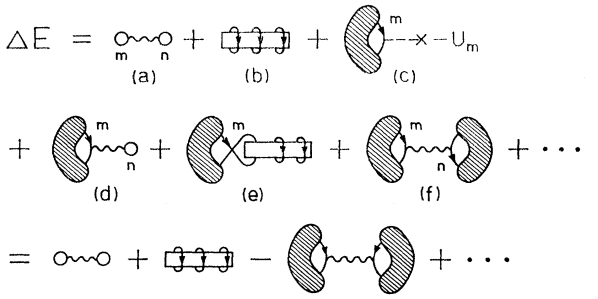

FIG. 8. Diagrams illustrating the overcounting problem.

Bloch[46,22] has shown that this overcounting problem can be solved in a very clean and simple manner. His analysis shows that the Goldstone energy series is reproduced by a combination of three terms,

$$\Delta E=\Xi_B-\Xi_L+\Xi_C. \tag{6.6}$$

The argument depends only on the most basic topological features of diagrams containing self-energy insertions. The same argument leads to quite similar expressions for several other types of renormalized perturbation expansions, all in the context of quantum statistical mechanics.[22,46] These will be discussed briefly in Sec. VIII.

In the present context, Ξ_B is just the "naive" expression mentioned above, namely the sum of all irreducible skeleton diagrams with each line representing a complete propagator. This term becomes an ordinary function of all of the potentials and occupation probabilities,

$$\Xi_B=\mathfrak{D}(U,P). \tag{6.7}$$

The next term becomes

$$\Xi_L=\sum_m U_mP_m-\sum_b U_b(1-P_b). \tag{6.8}$$

This can be represented symbolically as the trace of the product of the mass operator and the complete propagator, thanks to the relation

$$\Xi_L=\sum_j\oint_{C_j}\frac{d\omega}{2\pi i}\frac{(\pm)M_j(\omega)}{\omega-E_j^0-M_j(\omega)}$$
$$\equiv\mathrm{Tr}M\mathcal{G}. \tag{6.9}$$

The index j runs over all the m's and all the b's. The contours C_j must enclose the poles at $E_j^0+U_j$, but must *exclude* all other poles of "$\mathcal{G}$". The plus sign in (6.9) is for the normally-occupied states m. A minus sign is needed for the intermediate states b because, according to the diagram rules, there is a sign change when a mass-operator diagram for M_b is "closed" to produce a

[46] C. Bloch, Physica **26**, S62 (1960).

skeleton diagram for ΔE. From topological arguments[47] it can easily be shown that Ξ_L is just twice the *true* expectation value of the basic two-body interaction v. In other words,

$$\tfrac{1}{2}\,\mathrm{Tr}M\mathcal{G}=\langle\Psi_g|v|\Psi_g\rangle. \tag{6.10}$$

The last term Ξ_C just corresponds to the diagrammatic expansion of Eq. (6.1), summed over all single-particle states. Thus,

$$\Xi_C=\sum_m U_m-\sum_b U_b. \tag{6.11}$$

The final expression for the interaction energy is therefore

$$\Delta E=\mathfrak{D}(U,P)+\sum_m U_m(1-P_m)-\sum_b U_bP_b. \tag{6.12}$$

It is interesting to note that the second term in (6.12) is just the same as the diagram in Fig. 8(c). The third term can be represented similarly.

From the practical standpoint, this elegant solution of the overcounting problem is not vitally necessary. Its greatest value lies in the insight it gives concerning the general structure of the series. We have seen, from the elementary discussion accompanying Fig. 8, that there are no terms in the final expression for E/N which are proportional to $\langle P_m\rangle_{\mathrm{av}}$ or $\langle P_mP_n\rangle_{\mathrm{av}}$, contrary to what one might have guessed from the most naive considerations. The leading overcounting correction is only of order $-\langle(P_m-1)(P_n-1)\rangle_{\mathrm{av}}\times(E_2/N)\approx-\kappa^2(E_2/N)\approx+0.5$ MeV, and the higher corrections are all much smaller. The discussion of corrections due to $P_b>0$ is entirely similar. There the elementary argument shows that the leading correction is $-\langle P_aP_b\rangle_{\mathrm{av}}\times(E_2/N)$, which is utterly negligible. For the liquid He^3 problem, however, these overcounting corrections are surely much larger. In this case the elegant closed form (6.12) may be useful as a convenient way of including many small but not entirely negligible higher order terms.

Applications of the Complete Propagators, Finite Nuclei

We have just seen that the use of complete propagators, as opposed to self-energy propagators, is not worthwhile for a conventional nuclear matter calculation. The labor of carrying the P's throughout a calculation cannot be justified in terms of increased accuracy. Instead, it is much more convenient to treat the small overcounting effects as perturbations.

The situation is very different for the case of a finite nucleus. Suppose, for example, that one wishes to calculate the proton density distribution. The correct formal procedure is to use the Thouless expansion for the true expectation value of the proton density operator. This series differs from that of the interaction energy ΔE by the fact that the density operator now appears somewhere within each diagram.

This special operator can now be used to resolve the ambiguity about which part of the diagram is the skeleton. The skeleton is the part containing this operator, and all the other mass-operator parts are insertions. This is similar to the case of Fig. 7, where the external lines were used to resolve the ambiguity.

Now that the skeleton is unique, there is no longer any possibility of overcounting. It is therefore clear that the convergence of the Thouless expansion is significantly improved by using complete propagators everywhere. The same argument applies for the expectation value of any other operator. We therefore conclude that the renormalized propagators optimize the convergence of the *total nuclear wave function*.[5] This is a much more sensitive criterion for the definition of the shell-model potential than can be obtained from energy considerations alone. This is why we consider the "saturation potentials" of Sec. IV to be significant for a theory of finite nuclei.

Another application should be mentioned. By definition, the "valence-interaction" diagrams of the degenerate formalism all have external lines. The discussion of Fig. 7 therefore applies directly, showing that it is worthwhile to dress all the *internal* lines of these diagrams by means of the complete propagators.

VII. MASS-OPERATOR VARIATIONAL PRINCIPLE

We have already mentioned in Sec. IV that U_b can be thought of as the *increase* in the energy of the "other" clusters due to the filling of state b by the "skeleton" process. The structure of the U_m insertions allows a similar interpretation. This represents the *loss* of interaction energy from the "other" clusters involving particle m, due to the vacancy of state m caused by the "skeleton" process. Since $U_b>0$ and $U_m<0$, it is clear that they both tend to increase the magnitudes of all the energy denominators, and thereby to reduce the binding energy contributions from all of the skeletons. This can be seen, for example, in Eq. (4.1). The potentials, therefore, represent a kind of competition between the various possible "modes" of correlation. This competition establishes a special kind of equilibrium within the system.

The formal statement of this equilibrium condition is that the renormalized expansion possesses a remarkable stationary property. Equation (6.12) expresses the interaction energy ΔE as an *ordinary* function of all the U's and P's. Bloch's topological analysis[46] shows that this function must be stationary with respect to small variations in any of the U's and P's. This can easily

[47] See, for example, A. Klein, *Lectures on The Many-Body Problem, Naples, 1962*, edited by E. R. Caianiello (Academic Press Inc., New York, 1962) and T. D. Schultz, *Quantum Field Theory and the Many-Body Problem* (Gordon and Breach Science Publishers, Inc., New York, 1964).

be checked directly. A simple inspection of the diagrams shows that

$$\frac{\delta(\Delta E)}{\delta U_m}=\frac{\delta \mathfrak{D}}{\delta U_m}+(1-P_m)=0, \tag{7.1}$$

and

$$\frac{\delta(\Delta E)}{\delta P_m}=\frac{\delta \mathfrak{D}}{\delta P_m}-U_m=0, \tag{7.2}$$

with similar results for U_b and P_b. The U's and P's are all determined by the mass operator, hence an equivalent statement is that ΔE is stationary with respect to small changes in the mass operator.

This stationary principle has an interesting history. It first appears in a quantized many-body formalism in the expansion of Lee and Yang[21] for quantum statistics. It is related to a whole heirarchy of similar results obtained earlier in classical statistical mechanics. The latter all stem from the fact that the entropy is maximized by the equilibrium-density distribution. The connections are discussed in Ref. 22. *Note added in proof.* At zero temperature, this can be related to the familiar Raleigh-Ritz variational principle. This has useful consequences for the theory of finite nuclei, although, as argued below, it does not appear to be useful for an infinite system. A report is in preparation.

It has been suggested that this stationary property should make a calculation of the nuclear-matter binding energy insensitive to the choice of the single-particle energies.[48] This deserves to be investigated. The stationary theorem would seem to assume (i) that the function $\mathfrak{D}(U,P)$ has been determined correctly, and (ii) that all except one of the U's and P's have been assigned their exact values. Now there are two sources of error in any practical calculation: (a) the selection of certain skeleton diagrams to define $\mathfrak{D}$ and M, and (b) the numerical calculation techniques. The approximations will invalidate both assumptions (i) and (ii), therefore the practical consequences of this principle require further examination.

One can gain some insight into the meaning of this variational principle by applying the formalism to the case of a single particle bound in a perturbed potential well. First of all, one must make sure that the prescription for identifying the self-energy insertions in an arbitrary diagram is unambiguous. For a one-body problem this requirement will only allow the propagator renormalization to be applied to a *single* one of the unperturbed states. (The *diagonal* elements of V, i.e. V_{jj}, can obviously be summed out for all states Φ_j. The nondiagonal elements are the ones which can lead to ambiguities.) In principle, any state can be chosen for this renormalization.

We shall choose the initial state Φ_0. The relevant formulas are then

$$U_0=M_0(U_0), \tag{7.3}$$

where

$$M_0(U)=\left\langle \Phi_0 \middle| V \sum_{n=0}^{\infty} \left(\frac{Q}{E_0+U-H_0}V\right)^n \middle| \Phi_0 \right\rangle, \tag{7.4}$$

and

$$P_0=\left[1-\frac{\partial M_0}{\partial U}\bigg|_{U_0}\right]^{-1}=|\langle \Phi_0|\Psi_g\rangle|^2. \tag{7.5}$$

These should be recognized as the formulas of Brillouin-Wigner perturbation theory. The interaction energy expression (6.12) becomes

$$\Delta E=P_0[M_0(U_0)-U_0]+U_0. \tag{7.6}$$

This is obviously stationary with respect to variations in P_0 and U_0, provided that Eqs. (7.3) and (7.5) are satisfied. Alternatively, one can regard the stationarity requirement as simply another way of stating Eqs. (7.3) and (7.5).

One can now see the purely formal nature of the stationary result. The statement is equally valid for *any* function $M_0(U)$, regardless of whether this function has been determined correctly for the *physical* system. In a many-body system one finds, similarly, that the variational principle is formally valid for *any* selection of skeletons to represent $\mathfrak{D}$ and M, as long as the same selection is used for both. In this sense the variational principle is rather trivial, since it tells us nothing about the accuracy of the final result for ΔE. It certainly must not be interpreted as a license to use crude approximations, in the hope that self-consistency will somehow suppress the error in the final ΔE.

Self-Consistency

Of course self-consistency is a good thing which one should strive for in any practical calculation. Experience has shown that if one makes a bad approximation somewhere in the calculation of the G-matrix elements, the error in the computed E/N is reduced when the approximate scheme of equations is solved self-consistently. This feature is quite understandable in terms of the one-body analogy. Consider Eq. (7.3), and imagine that one knows the exact solution U_0 corresponding to the physically correct function M_0. If one now falsifies M_0 by adding a function δM, the quantity $\delta M(U_0)$ will certainly *overestimate* the error δU that would result from a self-consistent solution of the new Eq. (7.3). This is simply because $\partial M(U)/\partial U$ is always negative. The improvement arising from self-consistency is essentially the same as the improvement resulting from the use of Brillouin-Wigner perturbation theory instead of Raleigh-Schrödinger perturbation theory. In the many-body system, the renormalized expansion replaces the initial problem by a coupled set of systems, each of which is treated by Brillouin-Wigner methods.

Let us try to judge how important self-consistency is in a practical nuclear matter calculation. The number of coupled equations necessary for a practical calculation can be greatly reduced through the use of Gaussian

[48] A. Klein, Phys. Rev. 121, 950 (1961).

integration techniques.[49] Carrying this idea to the limit, we can simplify the problem to a *single* equation of the form (7.3). Thus we shall think of calculating the diagonal G-matrix element for an "average pair" in the Fermi sea, and use this to calculate $\langle U_m\rangle_{\rm av}$, etc. We shall ignore U_b, P_b, and P_m, and also all the higher order clusters. The set of equations then reduces to

$$U=\rho G\equiv M(U). \tag{7.7}$$

The change in U due to a small error in the function M is

$$\delta U=\frac{\partial M}{\partial U}\delta U+\delta M=\delta M\left(1-\frac{\partial M}{\partial U}\right)^{-1}. \tag{7.8}$$

Of course we are really dealing with two-body interactions; thus

$$E_2/N=\tfrac{1}{2}M(U). \tag{7.9}$$

Comparing this with (4.1), we see that

$$\frac{1}{2}\frac{\partial M}{\partial U}=-\kappa. \tag{7.10}$$

Putting all this together, we obtain

$$\begin{aligned}\delta(E_2/N)&=\tfrac{1}{2}\delta M\left(1-\frac{\partial M}{\partial U}\right)^{-1}\\&=\tfrac{1}{2}\delta M(1+2\kappa)^{-1}.\end{aligned} \tag{7.11}$$

The factor $(1+2\kappa)^{-1}$ represents the reduction of the error due to self-consistency. For $\kappa=0.12$ this factor is 0.8. We conclude that self-consistency gives a noticeable improvement, reducing the error by something like 20%, but this is very far from being a cure-all for otherwise bad approximations. The concepts of stationarity and self-consistency do not spare one from the necessity of doing a careful job at each step of a practical calculation.

VIII. COMPARISON WITH OTHER FORMAL THEORIES

Bloch's review article[22] lists four distinct renormalized perturbation expansions for quantum statistical mechanics. These are (i) the Lee-Yang expansion,[21] (ii) that of Luttinger and Ward,[50] (iii) the "true occupation number" formulation of Balian, Bloch, and De Dominicis,[51,52] and (iv) "quasiparticle" formulation of Balian and De Dominicis.[52,53] All four of these have expressions analogous to (6.12), in terms of renormalized propagators, and all of them possess mass-operator variational principles. For all of these, as well as for the present expansion, one can say that the self-energy problem has been solved to all orders of perturbation theory.

We mention this to emphasize that "the" self-energy problem is not uniquely defined by mathematical considerations alone. The many-body problem differs from field theory in this regard, and this has frequently been a source of confusion. The choices among the various possible partial summations must be based on *physical* considerations. The reasons for our particular choices were discussed in Sec. V.

In a certain sense, the present expansion stands midway between the "true occupation number" formulation and the "quasiparticle" formulation. Our downgoing lines are weighted by the true occupation numbers for states inside the Fermi sea, whereas they have zero weight for the states outside. Similar statements apply to the upgoing lines.

The true-occupation-number formulation is the one most closely related to the original cluster expansion of classical statistical mechanics. It reduces to the latter in the high-temperature limit, but it diverges very badly at low temperatures. On the other hand, the quasiparticle formulation is designed to give a convenient description of the low-temperature behavior. It leads to thermodynamic expressions of just the same form as in the Landau theory. The Fermi surface is treated very nicely, but it is not clear whether this can give an adequate description of the short-range few-body correlations.

The similarity to the expansion of Lee and Yang and of Mohling was mentioned in Sec. III. True occupation numbers also appear in these expansions, but the states inside and outside of their multiple collision operators or reaction matrices are not given the same treatment. It appears that their renormalized propagator techniques have not been exploited as fully as possible.

The Luttinger-Ward expansion is the one most closely analogous to renormalized field theory. Like the quasiparticle formulation, it also focuses attention on the neighborhood of the Fermi surface, and it also provides a formal justification for the Landau theory.

Comparison with the Green's-Function Theory of Nuclear Matter

It is also interesting to compare the present formulation with Puff's theory of nuclear matter.[54] This is

[49] K. A. Brueckner and J. L. Gammel, Phys. Rev. **109**, 1028 (1958).

[50] J. M. Luttinger and J. C. Ward, Phys. Rev. **118**, 1417 (1960). For an alternative development leading to essentially the same expansion, see A. Klein, Refs. 47, 48, and Phys. Rev. **121**, 957 (1961). This expansion has been related to the Landau theory by P. Nozieres and J. M. Luttinger, Phys. Rev. **127**, 1423 (1962); **127**, 1431 (1962).

[51] R. Balian, C. Bloch, and C. De Dominicis, Nucl. Phys. **25**, 529 (1961); **27**, 297 (1961).

[52] C. Bloch, R. Balian, and C. De Dominicis, Physica Suppl. **26**, 62 (1960); **26**, 94 (1960); also *Lectures on Field Theory and the Many-Body Problem*, edited by E. R. Cainaniello (Academic Press Inc., New York, 1962).

[53] R. Balian and C. De Dominicis, Nucl. Phys. **16**, 502 (1960); Compt. Rend. **250**, 3285 (1960); **250**, 4111 (1960); C. De Dominicis, thesis, Paris, 1961 (unpublished).

[54] R. D. Puff, Ann. Phys. (N. Y.) **13**, 317 (1961); D. S. Falk and L. Wilets, Phys. Rev. **124**, 1887 (1961); D. S. Koltun and L. Wilets, *ibid.* **129**, 880 (1963); J. C. Reynolds and R. D. Puff, *ibid.* **130**, 1877 (1963); J. C. Reynolds, *ibid.* **130**, 1891 (1963); A. S. Reiner, *ibid.* **133**, B1105 (1964); C. B. Duke, *ibid.* **136**, B59 (1964); R. D. Puff, A. S. Reiner, and L. Wilets, *ibid.* **149**, 778 (1966).

based on the Martin-Schwinger heirarchy of Green's function equations of motion.[55] In common with the Lee-Yang expansion, the attempt is made to derive all of the necessary formulas without ever resorting to an expansion in powers of the bare interaction v.

The most significant difference between this theory and ours is the fact that the Green's-function theory expresses the total energy as the sum of the *true* kinetic energy plus the *true* potential energy,

$$E=\langle\Psi_0|T_{\rm op}|\Psi_0\rangle+\langle\Psi_0|v|\Psi_0\rangle. \tag{8.1}$$

The true kinetic energy is given by

$$\langle\Psi_0|T_{\rm op}|\Psi_0\rangle=\sum_m T_m P_m+\sum_b T_b P_b. \tag{8.2}$$

We recall that a hard-core potential leads to an extremely long "tail" in the momentum distribution,

$$P_b\propto|\langle\mathbf{k}_b|\zeta\rangle|^2. \tag{8.3}$$

This means that a really careful calculation of (8.2) would be very difficult. Another point to notice is that the quantities P_m [or $(1-P_m)$] and P_b enter linearly in (8.2), as compared to a quadratic dependence in our final expression (6.12). This means that the P's need be calculated to considerably higher accuracy in Puff's approach then in ours, for the same accuracy of the final result.

As is well known, the true potential energy is related to the interaction energy ΔE, also called the "model" potential energy, by an integration over the coupling constant.[47] The true potential energy may be expressed in the form $\frac{1}{2}\Xi_L=\frac{1}{2}\,\mathrm{Tr}M\mathcal{G}$. Because of the close relation of Puff's methods to field theory, it would probably be more appropriate to compare his expressions with the $\frac{1}{2}\,\mathrm{Tr}M\mathcal{G}$ term in the Luttinger-Ward expansion, or in the expansion of Klein,[47,48] than with our "true" expression (6.8).

In practice, very little is yet known about the higher order approximations. Puff's original approximation neglects the exclusion principle in the intermediate states of his reaction matrix, although Falk and Wilets[54] have identified some correction terms which correspond to an exclusion effect. A rather discouraging feature of his approximation is that it neglects all of the terms arising from the "tail" of the momentum distribution. For example, the $\sum_b$ in (8.2) is neglected. This may not have as serious an effect as appears at first sight, since the corresponding potential-energy terms are also neglected. The most disturbing consequence is that the number of particles is not conserved, i.e.,

$$\sum_m P_m < N. \tag{8.4}$$

Puff has compensated for this by introducing an artificially large Fermi momentum.

In higher order approximations one would eventually be forced to deal with the full complexity of the spectral weight functions. One would then have to compute a *continuous* function $A_k(\omega)$ for *each* of the single-particle orbitals k. These functions contain a great deal of information, but much of this is irrelevant for the properties of the ground state. Thus the method appears rather inefficient.

Quite apart from the uncertainties associated with the present approximations of this approach, we feel that the use of the "true" energy expression (8.1) is a great disadvantage as compared to the "model" quantity ΔE. The advantages of the "model" description are: (1) The degenerate version of this model formalism[9–13] corresponds quite directly to the usual shell-model concepts. (2) The model kinetic energy (or unperturbed shell-model energy $\langle H_0\rangle$) is trivial to calculate, in contrast to the true kinetic energy. (3) The true kinetic and potential energies have considerably larger magnitudes than the corresponding model quantities, thus the true quantities must be calculated to relatively higher accuracy in order to achieve the same accuracy for the final E/N. (4) Finally, the model energy expression (6.12) is much less sensitive to errors in the computed values of the P's. Further comparisons between the "true" and "model" descriptions may be found in Prange and Klein[56] and in Ref. 13.

If one considers the nonperturbative aspect of Puff's theory to be important, it might be worthwhile to attempt a similar nonperturbative theory within the model description. This could probably be done by developing the theory of Kümmel.[57]

IX. SUMMARY AND CONCLUSIONS

The object of this paper has been to find a systematic and physically reasonable scheme for rearranging the higher order terms in the Brueckner-Bethe-Goldstone theory of nuclear matter. There were two motivations for this study: (a) to explore and develop the consequences of Bethe's three-body cluster idea, and (b) to obtain a satisfactory theory of finite nuclei. The first of these focuses attention on the off-energy-shell problem and the role of the healing distance. The second problem emphasizes the need for a mass operator which is well defined, to all orders of perturbation theory, in a physically meaningful way. Taken together, these considerations lead to a unique choice of partial summations. The latter can be applied consistently throughout the *entire* series, and one thereby obtains a new form of renormalized many-body perturbation theory. Its distinctive feature, as compared with other renormalized perturbation theories, is that it optimizes the treatment of the short-range correlations between particles which are deep within the Fermi sea. It is well established that the bulk properties of nuclear systems are determined almost entirely by these correlations.

[55] P. C. Martin and J. Schwinger Phys. Rev. **115**, 1342 (1959).

[56] R. Prange and A. Klein, Phys. Rev. **112**, 1008 (1958).

[57] H. Kümmel, in *Lectures on the Field Theory and the Many-Body Problem*, edited by E. R. Caianiello (Academic Press Inc., New York, 1962).

When more than two particles are excited from deep within the Fermi sea, the energy denominators tend to be very large. This off-energy-shell effect greatly enhances the repulsive hard-core contribution to the G-matrix elements. On the other hand, there are many instances where the topology of a diagram permits a generalized time-ordering factorization, so that certain parts of the diagram may be evaluated "on the energy shell" with respect to the remainder of the diagram. The difference in the behavior of interactions on and off the energy shell is so striking that we have adopted this as the primary criterion for rearranging the linked-cluster series. This effect is intimately related to the hard core, and hence to the short-range correlations.

The *first* partial summation consists of grouping together all Goldstone diagrams which have the same structure in terms of irreducible compact parts (ICP's). Most simply, an ICP is a part of a diagram which can be "factorized" to place it entirely on the energy shell with respect to the remainder of the diagram. In this way all off-energy-shell effects are concealed within the interiors of the various ICP's. For two or three particles, the ICP's are just the usual G-matrix and Bethe's three-body cluster, respectively. More generally, they closely resemble the multiple-collision operators of Lee and Yang.

Self-consistent single-particle potentials are introduced by means of a *second* partial summation. The previous summation forces us to adopt a particular choice of self-energy insertions. These are just the insertions which can be placed entirely on the energy shell. Their sum is said to define an on-energy-shell mass operator M^{on}.

A curious and very fortunate feature of this mass operator is that it leads to occupied-state potentials which are all strongly attractive, as in previous formulations of nuclear matter theory, but the intermediate-state potentials are all *positive*. This automatically places a lower bound of quite large magnitude (>100 MeV) on *all* of the energy denominators. In the language of the reference-spectrum method,[15] this ensures that the γ's are all quite large, and hence that the two-body correlations must heal quite rapidly. This also helps to make the off-energy-shell effects quite striking. The net effect is to guarantee that the spatial correlations within *and between* the many-body ICP's are all of quite short range, so that one is indeed dealing with "compact clusters." The initial assumption of strong off-energy-shell effects is therefore internally consistent. This strengthens our confidence that this is the most satisfactory way to handle the correlations between particles deep in the Fermi sea. The most important consequence is that the entire compact-cluster series can be ordered in terms of a small parameter κ, which turns out to be of order 10%.

It is noteworthy that this κ is essentially the same as the small parameter of the Jastrow cluster expansion. Day[58] has recently demonstrated a close connection between the three-body Bethe-Faddeev wave function and the corresponding Jastrow wave function which was used by Moszkowski.[7] It would be interesting to pursue this comparison further. It appears quite likely that the Jastrow expansion is simply a semiclassical approximation to the present one. The relation is obscured somewhat by the fact that the Jastrow method is based on the "true" description, which involves the true expectation values of the kinetic and potential energies, whereas the present method is based on the "model" description, $E=E_0+\Delta E$. We have argued that the model description provides the most convenient framework for a really detailed theory of nuclear systems.

The rapid decrease in the magnitudes of the first few terms of our expansion is physically reasonable, because the binding energy is dominated by the short-range correlations. But the true wavefunction also contains long-range correlations (BCS correlations for example), and these are artificially suppressed by the very large energy denominators. The existence of BCS correlations is probably enough to make the expansion diverge asymptotically (and there are also other reasons for suspecting an asymptotic divergence), but this in itself is not a serious drawback. This expansion should be satisfactory for binding-energy calculations, at least for infinite nuclear matter, because the BCS and other long-range correlations contribute so little here.

On the other hand, one would like to have a more general theory in which the long-range effects could be studied in detail. Suitable formulations can be constructed by applying the present partial summations to the degenerate linked-cluster expansion.[9–13] The basic idea is to split the set of unperturbed N-body eigenstates (Slater determinants) into two parts. The low-lying states are handled by the usual configuration-mixing approach in which one diagonalizes a secular matrix. The higher configurations are brought in through the linked-cluster expansion for the effective interaction of the secular problem.

It is obvious that this type of approach is needed for a real nucleus with only a few valence particles beyond closed shells.[59–61] It should also work when there are many valence particles. (This has been suggested before,[62,63] but at the time there was no adequate degenerate perturbation theory.) In this case one cannot hope to solve the secular equation exactly. But approximate solutions may be obtained by using the techniques of the BCS and random-phase theories, or even by a

[58] B. D. Day, Phys. Rev. **151**, 826 (1966).
[59] K. A. Brueckner, R. J. Eden, and N. C. Francis, Phys. Rev. **99**, 76 (1955).
[60] H. A. Bethe, Phys. Rev. **103**, 1353 (1956).
[61] J. F. Dawson, I. Talmi, and J. D. Walecka, Ann. Phys. (N. Y.) **18**, 339 (1962).
[62] K. A. Brueckner, in *Proceedings of the International Conference on Nuclear Structure, Kingston, Canada, 1960* (The University of Toronto Press, Toronto, Canada, 1960), p. 86.
[63] J. S. Bell, in *Lectures on the Many-Body Problem*, edited by C. Fronsdal (W. A. Benjamin and Company, New York, 1962).

second application of linked-cluster perturbation methods, depending on which long-range effects are being considered.

This approach makes explicit use of the logical continuity between conventional shell-model techniques and the treatment of the Fermi surface in infinite systems. A rather similar viewpoint has been taken by Migdal, who is applying the techniques of the Fermi liquid theory to shell-model calculations.[64] We are suggesting instead that a many-body formalism which was originally developed for the shell model be extended to infinite systems. By this means it may eventually be possible to calculate all of the semiphenomenological parameters of Landau and Migdal from first principles.

It is interesting that true single-particle occupation probabilities occur in a simple way throughout the present expansion. This happens because they are directly related to the on-energy-shell mass operator. One obtains the rather paradoxical result that these true occupation numbers are important for a finite system but not for an infinite system. They are not important in the infinite case because, in the final energy expression, almost all of their effect is compensated by "overcounting corrections." Their residual effect is so small (or order $\frac{1}{2}$ MeV) that it is much more convenient to regard this as a perturbation.

The renormalized probabilities are important in the finite case because they lead to a significant improvement in the total wave function. They do this mainly by improving the one-body orbitals. They introduce repulsive terms into the shell-model potential, and these terms increase more rapidly with the density than do the corresponding attractive terms. These terms clearly tend to bring about saturation, and we have therefore called them "saturation potentials."[5]

We have not yet referred to the generalized Brillouin condition,[65,66] which states that the *total* amplitude for a single-particle excitation should vanish. It is worthwhile to have the shell-model potential satisfy this condition since this will obviously improve the convergence of the theory. Fortunately, it is very easy to incorporate this into the theory. A much more difficult problem is to ensure that this shell-model potential is Hermitian. This will be discussed in a later paper. One should note that this theory of the shell-model potential, based on optimizing the convergence of the wave-function expansion, does not make any reference to variational arguments or to the physically observable removal energies. The view that the one-body potential should be regarded as a "free parameter," to be used to optimize the rate of convergence, has long been advocated by Bethe.[60]

Our single-particle energies are *not* the removal energies. This is consistent with most previous discussions of "rearrangement" effects.[67] One important consequence is that the velocity dependence of our shell-model potential should be quite different from that deduced from the experimental removal energies. There are indictions that the experimental effective mass is close to the real mass, or perhaps even larger than the real mass.[68,69] This is understandable from an examination of the rearrangement terms corresponding to the present theory.[5] These terms will be discussed more fully elsewhere, in connection with the degenerate formalism.

There is a good reason why the physical removal energies should not be used in a theory of nuclear binding energies. Except for the states just at the Fermi surface, the removal energies are all complex. (Even complex energies are inadequate to describe the propagation of particles or holes far from the Fermi surface.) We feel that complex numbers should be avoided in a theory of the bound many-body ground state. Some authors have proposed using just the real parts of the removal energies,[4,6] but this is a rather *ad hoc* prescription. It has also been suggested that one should keep track of the imaginary parts of the removal energies at all stages in a theory of the ground state.[70] This would make practical calculations more complicated. Besides, it is far from clear whether the resulting ground-state energy would be real.

The present intermediate-state potentials turn out to be extremely small, of order +1 MeV. For practical nuclear matter calculations they may simply be ignored. This is a great simplification compared to previous treatments of these potentials,[71] but of course there is a price to pay. One must now do a separate calculation of the three-body cluster energy. This approach has been advocated for some time by Brown,[72] both with regard to the convergence problem and as a very convenient simplification for G-matrix calculations in the shell model. In a later paper we shall argue that this simple and useful result may require modification in the nuclear surface region, due to a subtle nonlocal effect. Stated most simply, this comes from the requirement that the intermediate orbitals must all be orthogonal to the occupied orbitals.

For practical nuclear matter calculations, the intermediate-state potentials and occupation probabilities are both entirely negligible. The renormalization of the

[64] A. B. Migdal, in Proceedings of the International School of Physics "Enrico Fermi," Course 36, Varenna, 1965 (to be published).
[65] R. K. Nesbet, Phys. Rev. **109**, 1632 (1958).
[66] P. O. Löwdin, J. Math. Phys. **3**, 1171 (1962).
[67] K. A. Brueckner, Phys. Rev. **97**, 1353 (1955); D. J. Thouless, Phys. Rev. **112**, 906 (1959); P. Mittelstaedt, Nucl. Phys. **17**, 499 (1960); K. A. Brueckner and D. T. Goldman, Phys. Rev. **117**, 207 (1960); K. A. Brueckner, J. L. Gammel, and J. T. Kubis, *ibid.* **118**, 1438 (1960).
[68] G. E. Brown, J. H. Gunn, and P. Gould, Nucl. Phys. **46**, 598 (1963).
[69] B. L. Cohen, Phys. Rev. **130**, 227 (1963).
[70] D. J. Thouless, Phys. Rev. **114**, 1383 (1959).
[71] See Refs. 15, 17, 49, and also D. W. L. Sprung, Ann. Phys. (N. Y.) **31**, 342 (1965); S. A. Coon and J. Dabrowski, Phys. Rev. **140**, B287 (1965).
[72] T. T. S. Kuo and G. E. Brown, Nucl. Phys. **85**, 40 (1966); G. E. Brown, Unified Theory of Nuclear Models, 2nd edition (to be published).

occupied-state probabilities is *not* small, but its effect on the binding energy is so small that it is best regarded as a perturbation. In anticipation of the finite case we discussed the first four terms (U_2, U_3, U_{2S}, and U_{3S}) in the expansion for the occupied-state potentials. The last three of these terms are all fairly small, and there is probably considerable cancellation between them. It should be quite sufficient to treat these terms as perturbations, with due allowance for overcounting. The self-consistency part of a nuclear matter calculation then need only involve U_2. This is simpler than in most previous formulations.

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APPENDIX: MAGNITUDES OF THE COMPACT CLUSTERS

We wish to demonstrate that the κ of (4.2) is indeed the small parameter of the expansion. This requires some interpretation, because the result is not a simple Taylor series in κ. The best one can say is that the general order of magnitude of each term can be characterized by a definite power of κ. This is quite analogous to the rather complicated way the corresponding small parameters occur in the Jastrow expansion and in the classical virial expansion for imperfect gases. We shall begin with a rather detailed discussion of the simplest class of diagrams, those consisting of only a single ICP. This is to illustrate some of the other considerations which determine the magnitudes, in addition to the number of κ's. The identification of "factors" of κ is then discussed for the general case.

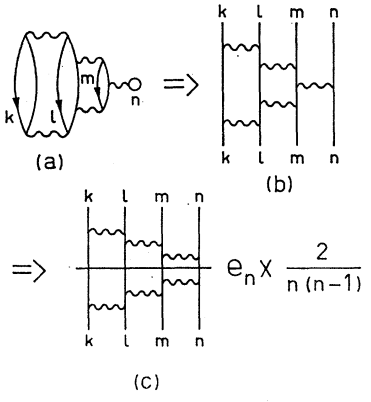

FIG. 9. Analysis of a typical diagram containing only a single irreducible compact part.

Diagrams With One Irreducible Compact Part

Consider the Goldstone diagram in Fig. 9(a). This is the simplest contribution to the $n=4$ compact cluster. By comparing this with the closed part on the right-hand side of Fig. 4(c), one can easily see that the order of magnitude of this diagram is

$$\kappa^{n-2}\rho\langle G_n\rangle. \tag{A1}$$

Here $\langle G_n\rangle$ denotes a matrix element [the middle interaction in Fig. 9(a)] whose energy denominators involve excitations of all n particles. Note that this diagram is of order G^{2n-3}. The effect of including all the other Goldstone diagrams of the same order (and their exchanges) which belong to this same compact cluster is mainly to alter the statistical weights for the partial waves of the various G matrices in Fig. 9(a). This was shown in detail by Rajaraman[39] for the case $n=3$. The inclusion of all the higher order Goldstone diagrams of this compact cluster then acts mainly to reduce the strength of the hard-core contribution to $\langle G_n\rangle$.

In a naive extension of Bethe's analysis to n particles, it can readily be seen that this core contribution will be reduced by a factor of $\binom{n}{2}=\frac{n(n-1)}{2}$, the number of distinct pairs which can be formed out of n particles.[73] This may not be completely correct, because we have not analyzed the spurious terms which must be explicitly subtracted out of the n-body Bethe-Faddeev wave function. But these spurious terms must also have similar core-reduction factors, so the present argument should suffice for order-of-magnitude purposes.

According to the reference-spectrum method,[15]

$$\langle G_n\rangle=\langle\phi|v|\psi_n\rangle\approx(\hbar^2/M)\langle\phi|(\gamma_n{}^2-\nabla^2)|\zeta_n\rangle$$
$$=e_n\langle\phi|\zeta_n\rangle\approx e_n\int|\zeta_n(\mathbf{r})|^2d\tau. \tag{A2}$$

There is not much error from replacing $\langle\phi|$ by $\langle\zeta_n|$ in the last step. These quantities are identical inside the hard core, while the large value of $\gamma_n{}^2$ ensures that ζ_n heals quite rapidly beyond the core. This falsifies the attractive contribution to $\langle G_n\rangle$, but we shall treat that more carefully below. For the moment, we shall replace e_n, the n-particle excitation energy, by n

[73] I am indebted to Dr. C. W. Wong for this observation.

times a typical single-particle excitation,

$$e_1 \approx (\hbar^2/2M)[(\pi/2c)^2 - 0.6k_F^2] + \langle U(b)\rangle_{\rm av} - \langle U(m)\rangle_{\rm av}$$
$$= [(2.6)^2 - 0.6]T_F + 70 \text{ MeV} = 300 \text{ MeV}. \quad \text{(A3)}$$

For $n=2$, the hard-core repulsive contribution is about half as strong as the attractive outer contribution (see Table III of BBP); thus

$$\rho\langle G_2\rangle_{\rm core} \approx -\tfrac{1}{2}\rho\langle G_2\rangle_{\rm outer} \approx -\rho\langle G_2\rangle. \quad \text{(A4)}$$

Now the magnitude of $\rho\langle G_2\rangle$ is $2(E_2/N) \approx -73$ MeV. We shall assume that the attractive outer contribution is roughly independent of n, therefore

$$\rho\langle G_n\rangle_{\rm outer} \approx \rho\langle G_2\rangle_{\rm outer} \approx -146 \text{ MeV}$$
$$\approx -4\kappa e_1. \quad \text{(A5)}$$

The core repulsion will be scaled down by a factor of $\binom{n}{2}$, as described above;

$$\rho\langle G_n\rangle_{\rm core} \to \frac{2}{n(n-1)} \times n e_1 \kappa, \quad \text{(A6)}$$

so that finally

$$\rho\langle G_n\rangle \to -\kappa e_1\left(4 - \frac{2}{n-1}\right). \quad \text{(A7)}$$

The statistical weights can be guessed as follows. We are dealing with correlations of quite short range, so there should be very little contribution unless the $n(n-1)/2$ different pairs can all interact in relative S states. Because of antisymmetry, this can only happen when the particles all begin in different spin-isospin states. The weights are therefore $w_2=\frac{3}{4}$, $w_3=\frac{3}{4}\times\frac{1}{2}$, and $w_4=\frac{3}{4}\times\frac{1}{2}\times\frac{1}{4}$. The contributions for $n>4$ should be very small, quite apart from the κ^{n-1} factor, because some of the pairs must begin in relative P states. In applying these statistical weights, we must also remember that κ, as defined in (4.2), already includes a factor of $w_2=\frac{3}{4}$.

Putting this all together, we obtain

$$E_n/N \approx -w_n(\tfrac{4}{3}\kappa)^{n-1} e_1\left(4 - \frac{2}{n-1}\right). \quad \text{(A8)}$$

The results are

$$E_2/N = -2\kappa e_1 = -72 \text{ MeV},$$
$$E_3/N = -2\kappa^2 e_1 = -8.6 \text{ MeV},$$

and

$$E_4/N = -(20/27)\kappa^3 e_1 = -0.38 \text{ MeV}.$$

Note that these results are all attractive. The hard-core repulsion has been strongly suppressed relative to the outer attraction.

These estimates are all somewhat too large. The $n=2$ case requires an extra factor of $\frac{1}{2}$, as in Hartree-Fock theory, because of the special symmetry of the E_2/N diagram. For the other cases one should note that the appropriate κ_n, for correlations whose energy denominators involve n-particle excitations, is considerably smaller due to the rapid healing. The asymptotic value for large n is determined by the hard-core volume,

$$\kappa_{n\to\infty} = \tfrac{3}{4}\rho \times \frac{4\pi}{3} c^3 = 0.05, \quad \text{(A9)}$$

for $c=0.45$ F. Another point to consider is that *at least* $\frac{1}{4}$ of $\langle G_2\rangle_{\rm outer}$ arises from the tensor force in triplet-even states. This will be strongly suppressed for $n>2$, both because of the off-energy-shell effect and because of the more complicated geometry. In this connection we recall that about $\frac{1}{3}$ of our estimate for κ was attributed to the subsidiary $^3D_1$ wave. (This is the analogue of the deuteron D wave.) From these considerations it should be reasonable, for $n>2$, to (a) multiply the outer contribution (A5) by a factor $\frac{3}{4}$, and (b) decrease the $n-2$ factors of κ which derive from (A1) from 0.12 to 0.08. The results are then $E_2/N=-36$ MeV, $E_3/N=-3.8$ MeV, and $E_4/N=-0.12$ MeV.

One may object that a more careful study of the diagrams [see, for example, Eq. (7.14) of BBP] shows that the appropriate e_n for (A2) is *not* n times (A3) but is instead

$$e_n \to n\langle \Delta U\rangle_{\rm av} + (n-1)\langle \Delta T\rangle_{\rm av}$$
$$\approx n \times 70 \text{ MeV} + (n-1) \times 230 \text{ MeV} \quad \text{(A10)}$$

for $n>2$, while for $n=2$,

$$e_2 \to 2\langle \Delta U\rangle_{\rm av} \approx +140 \text{ MeV}. \quad \text{(A11)}$$

On the other hand, we have effectively attributed most of the core repulsion to the core interior term of the reference-spectrum method, whereas for small n the bulk of this repulsion actually comes from the *core boundary* term. It turns out that there is a strong compensation between these two neglects. The naive discussion of the core repulsion actually gives reasonably good estimates.

We have carried this discussion far enough to show how one can obtain reasonable magnitude estimates without going through a full analysis. But we have so far only considered diagrams composed of a *single* irreducible compact part.

General Argument

For a general diagram there is no point in attempting so much detail. We are interested simply in identifying the factors of κ. For this purpose, the main steps of the argument are summarized in the sequence (a), (b), (c) of Fig. 9. The general case brings in one new feature, however. Some of the hole-line summations may be restricted by momentum conservation.

The first step in the analysis of a general compact-cluster diagram is to select a single one of the lowest order Goldstone diagrams which it contains. (Any of the lowest order diagrams will suffice; the exact choice is

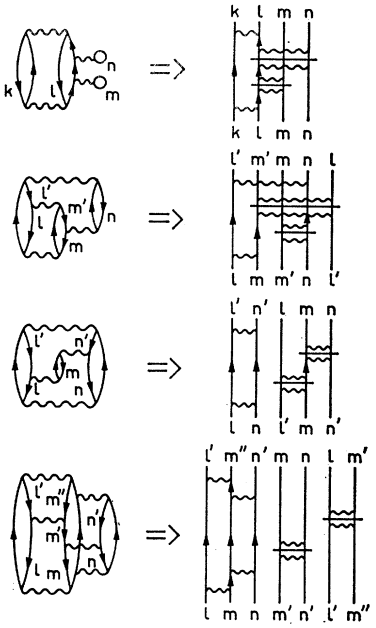

FIG. 10. Analysis of some typical diagrams containing more than one irreducible compact part.

unimportant.) The next step is to replace each downgoing line by a pair of upgoing external lines, as in Fig. 9(b).[74]

At this stage the diagram may contain several disconnected pieces. The number of these disconnected pieces will always be one greater than the number of hole-line summations which are restricted by momentum conservation. This follows directly from the topological features which lead to the momentum restrictions. We should now take note of the fact that we are actually interested in E/N, the energy per particle. In the present context the N^{-1} factor is equivalent to suppressing another one of the hole-line summations. The number of disconnected pieces is therefore the same as the *total* number of hole-line summations which are suppressed.

[74] This is essentially the diagram convention of Lee and Yang, Refs. 21, 22. Its use in the present context was suggested by R. Rajaraman, Ref. 20.

The diagram should now be examined to see if there are any continuous lines which encounter only a single G-matrix interaction during their journey from the bottom to the top of the diagram. If so, each of these "isolated" G-matrix elements should be "split open," as in (A2) and Fig. 9(c), to give an excitation energy multiplied by a factor of $\langle\zeta|\zeta\rangle$.

Let us begin with the simplest possible diagram, corresponding to E_2/N. The first (or left-hand) external line may be ignored, since this sum over occupied states is cancelled by the N^{-1} factor. Following the second (or right-hand) line from the bottom to the top, we encounter factors of ρ, $|\zeta\rangle$, an excitation energy e_2, and $\langle\zeta|$. These combine to give $\kappa\, e_2$.

Now consider a general connected part of an external-line diagram. Suppose that this part contains h external lines. The first of these corresponds to a factor of unity. Each succeeding line will add a factor of $\rho\langle\zeta|\zeta\rangle$, $\rho\langle\phi|\zeta\rangle$, or $\rho\langle\zeta|\phi\rangle$. For our purposes these are all equal to κ, so this connected part contributes a factor of κ^{h-1}. After analyzing all of the connected parts in this way, we obtain the desired over-all factor of $\kappa^{h'-1}$, where h' is the number of hole lines whose summations are *not* restricted by momentum conservation.

There will always be enough $|\zeta\rangle$ or $\langle\zeta|$ factors because, by construction, each line must get excited into an intermediate state and then eventually get de-excited again. There will be no superfluous ζ factors, because we have deliberately chosen one of the simplest or lowest order diagrams corresponding to the compact cluster. From the general rule that a diagram with n G's must have $n-1$ energy denominators, one can see that the above procedure will always lead to a single left-over factor of e, as required on dimensional grounds. The inclusion of all the other Goldstone diagrams will then simply add statistical weighting factors and core-reduction factors, all of which may be ignored here. Some further examples are shown in Fig. 10 to help fix these ideas. The straight horizontal lines illustrate where isolated G's have been split open.