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Linked-Cluster Expansions for the Nuclear Many-Body Problem*

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The Goldstone expansion is rederived by elementary time-independent methods, starting from Brillouin–Wigner (BW) perturbation theory. Interaction energy terms ΔE are expanded out of the BW energy denominators, and the series is then rearranged to obtain the linked-cluster result. Similar algebraic methods lead to the linked expansions for the total wave function (Hugenholtz) and the expectation value of a general operator (Thouless). Starting again with a degenerate version of BW perturbation theory, these methods are used to obtain the Bloch–Horowitz energy expansion, as well as the corresponding wave function, expectation-value, and transition-amplitude expansions. A "reduced" form of the Block–Horowitz expansion is described, and also a "completely linked" version. The latter is suggested as a tool for investigating superfluid phenomena in nuclear matter, and for establishing contact with the Landau theory of Fermi liquids. The physical interpretation of these expansions is carefully studied, especially with regard to nuclear applications, to determine how they handle such "physical" features as antisymmetry, self-energy effects, wave-function renormalizations, and the distinction between "true" and "model" single-particle occupation probabilities. The problem of a correct theoretical definition for the shell-model potential is carefully examined, and a specific theory is presented. These expansions are seen to form a convenient and very powerful set of tools for studying the structure of actual nuclei.

CONTENTS

I. INTRODUCTION

The Brueckner–Bethe–Goldstone theory of nuclear matter is now reaching the stage where it can be usefully applied in studies of actual nuclei.[1–23] To apply

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[1] References 2 to 14 deal with the formal theory of the nuclear ground state, including the effective two-body interaction. References 15 to 18 discuss the effective two-body interaction to be used in shell-model calculations. References 19 to 23 cover related topics and more phenomenological methods. For the theory of infinite nuclear matter, see Refs. 9, 11, 26, 47, 48, and also K. A. Brueckner and J. L. Gammel, Phys. Rev. **108**, 1029 (1958). See also two review articles: J. S. Bell and E. J. Squires, *Advances in Physics* (Phil. Mag. Suppl.) **10**, 211 (1961); A. G. Petschek, Ann. Rev. Nucl. Sci. **14**, 29 (1964). A very extensive review has also been given by K. Kumar, *Perturbation Theory and the Nuclear Many Body Problem* (North-Holland Publ. Co., Amsterdam, 1962).

[2] K. A. Brueckner, J. L. Gammel, and H. Weitzner, Phys. Rev. **110**, 431 (1958).

[3] K. A. Brueckner and D. T. Goldman, Phys. Rev. **116**, 424 (1959).

this theory, one should have a clear and thorough understanding of the basic mathematical tools, the linked-cluster expansions for the total energy, the total wave function, and the expectation value of a general operator. Unfortunately, these expansions have been surrounded by a certain aura of mystery, due to the fact that they were derived by methods rather foreign to studies of nuclear structure. The large body of linked-cluster literature has not sufficiently clarified their relation to the comparatively elementary quantum methods which are the standard tools for most nuclear structure studies. The main purpose of this paper is to show that essentially all of the basic time and temperature-independent linked-cluster results, including some which have not appeared previously, can be obtained by rather elementary algebraic methods.[24] This may not be the simplest or the most elegant approach, but it is a surprisingly powerful one, and it serves to emphasize the physical meaning of the results. It establishes an immediate contact with shell-model concepts, and it should therefore be fruitful in suggesting how these concepts are modified by nuclear-matter theory.

The present algebraic methods are closely related to those used in Brueckner's original investigation,[25,26] in which he explicitly demonstrated the cancellation of unlinked terms in the first few orders of Raleigh–Schrödinger (RS) perturbation theory. He observed that this cancellation depends on various algebraic identities among the energy-denominator products. There are two basic differences in the present approach which permit all orders to be treated at once. First, the starting point is the Brillouin–Wigner (BW) perturbation theory, whose formal structure is much simpler than that of the RS expansion. Secondly, we use a "factorization theorem",[27] which expresses the required energy-denominator identities in a simple and general form.

For completeness, we mention other derivations which have appeared since the original studies of

[4] K. A. Brueckner, A. M. Lockett, and M. Rotenberg, Phys. Rev. **121,** 255 (1961); K. S. Masterson, Jr., and A. M. Lockett, Phys. Rev. **129,** 776 (1963); K. S. Masterson, Jr., in *Methods of Computational Physics,* B. Alder, S. Fernbach, and M. Rotenberg, Eds. (Academic Press Inc., New York, 1966), Vol. 6.

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[8] B. H. Brandow, Phys. Letters **4,** 8 and 152 (1963); B. H. Brandow, *Comptes Rendus du Congres International de Physique Nucleaire,* P. Gugenberger, Ed. (Paris, 1964), Vol. II, p. 295; also Ph.D. thesis, Cornell University (1964) (unpublished). See also Ref. 24.

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[10] B. D. Day, Phys. Rev. **136,** B1594 (1964).

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[27] L. M. Frantz and R. L. Mills, Nucl. Phys. **15,** 16 (1960); see also Ref. 29.

Brueckner[25,26] and Goldstone.[28] Most of these have extended the basic linked-cluster result in directions with which we are not concerned. Hugenholtz[29] and Bloch[30] have obtained the energy and wave-function expansions by studying the poles of the resolvent operator, $(z-H)^{-1}$. Coester[31] has used an algebraic method based on commutator brackets and the Heisenberg equation of motion in interaction representation. He proves the elimination of unlinked terms, but gives no further details. Coester and Kümmel[32] then obtained the same result using commutator brackets alone, without recourse to perturbation theory. Hubbard[33] has used an adiabatic method with Feynman propagators; i.e., with unrestricted time-ordering in the multiple-time integrals. His treatment of the time-dependent polarizability of an electron gas is very similar to quantum electrodynamics. (Incidentally, the elimination of unlinked terms, or "vacuum fluctuations," was first discussed by Feynman[34] in his study of quantum electrodynamics.) Klein and Prange[35] obtained the Goldstone expansion using Green's function methods. Matsubara,[36] Montroll and Ward,[37] and Bloch and De Dominicis[38] have exploited the analogy between the Bloch equation of quantum statistics and the time-dependent Schrödinger equation, to express the partition function in a form very similar to the Goldstone expansion. The latter is then recovered by extrapolating to zero temperature.[39] Brout[40,41] has accomplished the same thing by a very novel method employing the "semi-invariants" of mathematical probability theory. Thouless[42] discusses both the energy and partition-function expansions, using the methods of Ref. 30 in a particularly clear and simple form. References 38 and 40–42 also discuss the finite-temperature classical limit, the original linked-cluster expansion of Ursell, Yvon, and Mayer.

The wave-function and expectation-value expansions (due, respectively, to Hugenholtz[29] and Thouless[42,43]) have been known for some years now, but they have received very little attention. We emphasize the connections between these different linked-cluster expansions, as well as their relations with the *RS* and BW expansions. In searching for physical interpretations, we have found it helpful to consider all of the basic linked-cluster expansions (for energy, wave function, and general expectation value) on an equal footing. This clarifies the way they handle such "physical" features as antisymmetry, self-energy effects, wavefunction renormalization, and the relation between "true" and "model" single-particle occupation probabilities. We shall also consider the relative merits of linked-cluster and BW methods for few-body systems such as light nuclei. (Some of the early linked-cluster literature contained errors or ambiguities of order N^{-1}. It will be clear from our derivations that the modern results are correct for all N, even down to $N=1$.)

One of the most important problems for nuclear applications is the treatment of degeneracy. Bloch and Horowitz[44] have found a very elegant solution, by a method related to the highly abstract resolvent-kernel formalism of Hugenholtz and Van Hove.[29] The same result (and essentially the same derivation) was discovered independently by Day.[45] Their expansion has many interesting and useful features. In fact, its general structure immediately suggests the nuclear shell model. Their result is rederived here, as well as the corresponding wave function, expectation value, and transition-amplitude expansions, by the algebraic methods mentioned above. This provides a simple interpretation for their very important result. It also sheds some light on the practical problems of convergence. This expansion can be used to extend the Hartree–Fock theory to the degenerate case, as well as to the case of singular interactions. In lowest order, it agrees with the old arguments[46,47,17] that the effective two-body interaction for shell-model calculations is given by Brueckner's reaction matrix. In higher orders, it provides a systematic method for improving this approximation.

It was hoped that our elementary algebraic approach might reveal further possibilities for useful rearrangements and partial summations. The technique of putting certain insertions "on the energy shell"[48] (generalized time ordering) is examined more closely. (See also Ref. 9.) We have also found a "reduced" form of the Bloch–Horowitz expansion, and this is shown to be a useful simplification. Morita[49] has proposed a more drastic simplification, in the form of a "completely linked" version of the Bloch–Horowitz expansion.

[28] J. Goldstone, Proc. Phys. Soc. (London) **A239**, 267 (1957).
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[35] A. Klein and R. Prange, Phys. Rev. **112**, 994 (1958). See also the lectures by these authors in Ref. 32.
[36] T. Matsubara, Progr. Theoret. Phys. **14**, 351 (1955).
[37] E. W. Montroll and J. C. Ward, Phys. Fluids **1**, 55 (1958).
[38] C. Bloch and C. DeDominicis, Nucl. Phys. **7**, 459 (1958); and **10**, 181 (1959); C. Bloch, *Studies in Statistical Mechanics*, J. DeBoer and G. E. Uhlenbeck, Eds. (North-Holland Publ. Co., Amsterdam, 1965), Vol. III.
[39] There are difficulties connected with this extrapolation. For a clear and simple discussion of the problems, see A. Katz, Nucl. Phys. **43**, 128 (1963).
[40] R. Brout, Phys. Rev. **115**, 824 (1959).
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[42] D. J. Thouless, *The Quantum Mechanics of Many-Body Systems* (Academic Press Inc., New York, 1961).
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[44] C. Bloch and J. Horowitz, Nucl. Phys. **8**, 91 (1958).
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[46] K. A. Brueckner, R. J. Eden, and N. C. Francis, Phys. Rev. **99**, 76 (1955).
[47] H. A. Bethe, Phys. Rev. **103**, 1353 (1956).
[48] H. A. Bethe, B. H. Brandow, and A. G. Petschek, Phys. Rev. **129**, 225 (1963). This paper is referred to as BBP.
[49] T. Morita, Progr. Theoret. Phys. (Kyoto) **29**, 351 (1963).

(Bloch and Horowitz treat the particles beyond closed shells by a form of BW perturbation theory, and this leads to some unlinked-cluster terms.) This interesting possibility has been confirmed, and we describe the results in detail.[24] This is the true degenerate analog of Goldstone's expansion. It is useful whenever there are many valence particles to consider. As an extreme example, it appears to be well suited for studies of the superfluidity of nuclear matter. This problem can be regarded as a limiting case where the number of valence particles is infinite. This expansion should also be useful for attempts to calculate the parameters of the Landau theory of liquid He^3 from "first principles."[50]

Much insight into many-body systems has come from the use of Green's function techniques. These methods appear, at first sight, to be radically different from the perturbation methods discussed here. However, a number of useful relations between these two approaches can be established by means of the Bloch–Horowitz expansion and its "reduced" and "completely linked" versions. These expansions have the important property of separating the effects of the isolated closed-shell system from all of the *changes* due to the *physical* addition of valence particles (or valence holes). This separation is valid to all orders of perturbation theory. In contrast to Green's function methods, however, one deals from the outset with the eigenstates of the complete, fully interacting system. The valence particles enter directly as fully dressed quasi-particles, and renormalization effects appear in the formalism in a straightforward way.

It should be quite feasible to combine both approaches for a more general "two-stage" theory of Fermi-liquid systems having singular interactions. The first step is to use Brueckner and Bloch–Horowitz methods to handle the problems of singular potentials. The results of this stage can be expressed in the form of a "reduced Hamiltonian." In various contexts, this can correspond to the shell-model Hamiltonian, or to the reduced Hamiltonian of superconductivity theory, or to the phenomenological Hamiltonian which is assumed in the Landau theory. This reduced Hamiltonian refers only to the system's valence-particle degrees of freedom, and these could just as well be called the "quasi-particle" degrees of freedom. The problem of diagonalizing this Hamiltonian can then be tackled by whichever many-body technique is most appropriate for the particular case. This is the point at which Green's function methods might be convenient.

This approach leads to a concrete definition for what is meant by a Landau quasi-particle. It casts the Landau theory of liquid He^3 into the same mathematical framework as a conventional shell-model problem. (The logical similarities between these different physical problems have been emphasized especially by Migdal.[51]) It is important to distinguish between the problems of the low-lying excitations, which are observed experimentally, and the problems of the very high virtual excitations arising from a singular interaction. The degenerate perturbation expansions offer a *systematic* means for separating these problems, which are, after all, physically quite distinct. There are a number of objective reasons for believing that the high virtual excitations (or equivalently, the short-range correlations) can be handled most reliably by Brueckner-theoretic methods, at least for the nuclear many-body problem.[9] It remains to be seen whether these methods can be made quantitatively reliable for liquid He^3.

The presence of a strong short-range repulsion in the basic two-nucleon interaction requires that any perturbation expansion be carried to infinite order. This is equally true for the degenerate case of an open-shell nucleus. Thus we begin, in Sec. II, by discussing a form of degenerate perturbation theory which is easily expanded to infinite order. This is a generalization of the BW perturbation theory, and it retains much of the formal simplicity of that theory. This forms our starting point for the Bloch–Horowitz expansion, and it also provides some hints concerning a reasonable choice of "degenerate" states in any particular application. Section III contains a derivation of the Goldstone expansion for a particularly simple system—a single particle moving in an external potential. This serves to introduce the factorization theorem. It also illustrates some important relations between the BW, RS, and Goldstone expansions. Sections IV and V then deal with the nondegenerate (Goldstone) and degenerate (Bloch–Horowitz) energy expansions, including a "reduced" form of the latter. Section VI deals with wave functions, expectation values, and transition amplitudes. Section VII confirms Morita's arguments for a completely linked version of the Bloch–Horowitz expansion, and brings his program to completion. Possible applications of this formalism are discussed in Sec. VIII. Physical interpretations are examined in Sec. IX. Section X discusses the problem of a correct theoretical definition for the shell-model potential. Finally, we draw attention to an appendix on the diagram rules, since these have not always been spelled out in an unambiguous form. These are expressed here in a form convenient for nuclear applications—a combination of the rules given by Goldstone and Hugenholtz.

Section VII and parts of Sections V and VIII are considerably more difficult than the others. For a first reading, we suggest that one study Secs. II–IV carefully, skim over Secs. V and VI paying special attention to the discussions of (5.13) and (5.16), and then

[50] K. A. Brueckner and J. L. Gammel, Phys. Rev. **109**, 1040 (1958) [Errata: Phys. Rev. **121**, 1863 (1961)]; K. A. Breuckner, T. Soda, P. W. Anderson, and P. Morel, Phys. Rev. **118**, 1442 (1960); K. A. Brueckner, in *Many-Body Theory* (Tokyo, 1965), R. Kubo, Ed. (Syokabo and W. A. Benjamin, Inc., New York, 1966). See also Ref. 102.

[51] A. B. Migdal, *Proceedings of the International School of Physics "Enrico Fermi," Course 36* (Varenna, 1965), C. Bloch, Ed. (Academic Press Inc., New York, 1966).

proceed to Secs. IX and X. Reference 24 is also recommended as an easy introduction.

II. DEGENERATE PERTURBATION THEORY

Consider a very general quantum system, to be described by

$$H=H_0+V. \tag{2.1}$$

This need not be a "many-body" system. We begin as usual with

$$\Psi=\sum_i a_i\Phi_i, \tag{2.2}$$

$$(H-E)\Psi=0, \tag{2.3}$$

and

$$(H_0-E_i)\Phi_i=0, \tag{2.4}$$

from which one immediately obtains

$$(E-E_i)a_i=\langle\Phi_i\,|\,V\,|\,\Psi\rangle. \tag{2.5}$$

We then select a certain number d of the Φ_i's to span a "quasi-degenerate" subspace (model subspace) D. (Exact degeneracy is not required.) With this choice of D we associate a degenerate projection (model wave function)

$$\Psi_D=\sum_{i\epsilon D}a_i\Phi_i=P\Psi, \tag{2.6}$$

and a Green's function

$$\mathcal{G}=\sum_{i\notin D}\frac{|\,\Phi_i\rangle\langle\Phi_i\,|}{E-E_i}=\frac{Q}{E-H_0}, \tag{2.7}$$

so that (2.2) and (2.5) can be combined in the form

$$\Psi=\Psi_D+\mathcal{G}V\Psi. \tag{2.8}$$

It is now convenient to define a wave operator Ω by

$$\Psi=\Omega\Psi_D. \tag{2.9}$$

This corresponds to the nuclear model operator of Eden and Francis.[52] Similarly, we introduce a reaction matrix or "effective interaction,"

$$\mathcal{U}=V\Omega. \tag{2.10}$$

Substitution in (2.8) gives

$$\Omega=1+\mathcal{G}V\Omega, \tag{2.11}$$

and

$$\mathcal{U}=V+V\mathcal{G}\mathcal{U}. \tag{2.12}$$

Now (2.5) can be rewritten as

$$\begin{aligned}(E-E_i)a_i&=\langle\Phi_i\,|\,V\Omega\,|\,\Psi_D\rangle\\&=\sum_{j\epsilon D}\langle\Phi_i\,|\,\mathcal{U}\,|\,\Phi_j\rangle a_j.\end{aligned} \tag{2.13}$$

This is true for *all* states Φ_i, whether in D or not. In particular it holds for the a_i's in D, and these d equations can be grouped together to form a d-dimensional secular equation,

$$[H_0+\mathcal{U}(E)-E\mathbf{I}]\mathbf{A}=0. \tag{2.14}$$

This is the desired result.[53] Iteration of (2.12) gives a formal solution for $\mathcal{U}$ in terms of a perturbation series. Note that this reduces to familiar forms in several limiting cases: (a) to ordinary degenerate perturbation theory when V is weak; (b) to Brillouin–Wigner perturbation theory when D contains only one state, say Φ_0; and (c) to the usual matrix form of Schrödinger's equation when D is the entire Hilbert space.

This looks like the usual form of degenerate perturbation theory, except that it is now exact. All the "nondegenerate" states are concealed within $\mathcal{U}$. This effective interaction is generally well-behaved, even for a singular V. The true wave function vanishes wherever V is singular, and this is reflected in the behavior of Ω. (Of course one then needs a nonperturbative way to calculate $\mathcal{U}$.) This formalism can, at least in principle, provide a rigorous justification for the use of a "reduced Hamiltonian" $\mathcal{H}_D\equiv H_0+\mathcal{U}$ in problems as diverse as nuclear structure, superconductivity, and the Landau theory of Fermi liquids. (We shall return to these problems in Secs. VIII and IX.) This also shows the full generality of a phenomenon frequently observed in nuclear structure—the main effect of high-lying configurations is simply to "renormalize" the effects of the low configurations.

The convenience of having all "nondegenerate" states concealed in $\mathcal{U}$ is partly offset by the fact that this $\mathcal{U}$ depends on E, through (2.7). Bloch and Horowitz[44] have studied the analytic properties of the $d\times d$ matrix, $[H_0+\mathcal{U}(z)-zI]$, for complex z. Their most important result is that the eigenvalues [the E's of (2.14)] are all real. (A simple discussion of these analytic properties is given here in Appendix A.) The eigenvectors $\mathbf{A}$ are generally *not* orthogonal, because $\mathcal{U}(E)$ is Hermitian only when E is held fixed. Only when certain of the E's are identical, or when the $\mathbf{A}$'s (in other words, the Ψ_D's) differ in some conserved quantum number, can one assert that the $\mathbf{A}$'s are orthogonal. Of course the *total* Ψ's must be orthogonal, but their degenerate projections need not be. In practice one must use an iteration procedure: asume E, calculate $\mathcal{U}$, obtain a new estimate for the desired eigenvalue E, etc.[56] It could well be that the spread between the *desired* eigenvalues is so small, compared to a typical energy denominator in $\mathcal{U}$, that the E in $\mathcal{U}(E)$ might be

[52] R. J. Eden and N. C. Francis, Phys. Rev. **97**, 1366 (1955). See also Refs. 46, 47, and 17.

[53] This simple and convenient form of degenerate perturbation theory has received surprisingly little attention. The most extensive discussion is that of P.-O. Löwdin, J. Math. Phys. **3**, 969 (1962), where a number of earlier references are given. See also Refs. 44, 54, and 55. Note that our present derivation makes no assumption that V is "weak." The only expansion used has been that of Eq. (2.2).

[54] C. Bloch, Nucl. Phys. **6**, 329 (1958).

[55] J. Des Cloizeaux, Nucl. Phys. **20**, 321 (1960).

[56] Löwdin has shown (Ref. 53) that this simple iteration scheme does not always converge. In nuclear applications this problem can be avoided by using the methods of Sec. VII.

considered constant. In this approximation, then, the corresponding **A**'s (the model wave functions) would be orthogonal. This orthogonality problem is discussed further in Appendix D.

Presumably, D can be chosen such that this procedure converges reasonably well for that *subset* of the d eigenstates which one is particularly interested in. In nuclear physics one is usually content with just a few of the lowest E's for a given D. An example is a "pairing" calculation, where d could be very large. The choice of D should take account of all available insights, such as whether the states of interest are "collective" or not. This is just the familiar problem of choosing the right configurations.

For a weak V it would be reasonable to calculate $\mathcal{U}$ by iterating (2.12). A satisfactory D might then be found simply by requiring that the denominators $(E-E_i)$ be much larger than the elements V_{ij}, for all $i \notin D$. This criterion should also apply to more strongly interacting systems, provided that (a) the single elements V_{ij} are replaced by suitable partial summations, and (b) that "self-energy" effects are properly identified and included in H_0. When V is singular, one is forced to deal directly with the integral equation (2.12). This amounts to treating an infinite number of the Φ_i's simultaneously. The amplitudes for most of these Φ_i's will be very small, however, so it should suffice to treat them only in some "average" manner.[57] But regardless of whether V is strong or weak, one must expect poor convergence or even diverging approximations for $\mathcal{U}$ unless all of the "large" a_i's are included in the column vector **A**. For large or strongly interacting systems it often turns out that $|\langle\Phi_i|\Psi\rangle| \ll 1$ for *all* i (assuming $\langle\Psi|\Psi\rangle=1$), so the formal statement of this criterion for D must be

$$|\langle\Phi_i|\Psi\rangle| \ll \text{maximum of } |\langle\Phi_j|\Psi\rangle|, \quad i \notin D. \quad (2.15)$$

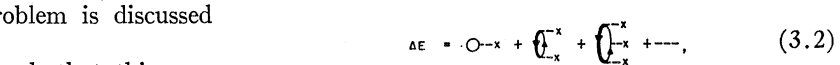
This is discussed further in Sec. IX.

III. ONE-BODY SYSTEM, FACTORIZATION THEOREM

We shall first derive the Goldstone expansion for the particularly simple case of a system containing only one particle. This illustrates a number of relations between the Brillouin–Wigner (BW), Raleigh–Schrödinger (RS), and Goldstone expansions, and it also serves to introduce the factorization theorem. We begin with the BW expansion,

$$\Delta E = E - E_0 = \langle\Phi_0|\mathcal{U}|\Phi_0\rangle$$
$$= \langle\Phi_0|V+V\mathcal{G}V+V\mathcal{G}V\mathcal{G}V+\cdots|\Phi_0\rangle, \quad (3.1)$$

which follows from (2.14) when the "degenerate" space D contains only the single state Φ_0. The terms of this expansion are represented by closed-loop or "vacuum" diagrams,



(3.2)

where the heavy downgoing line indicates the presence of the perturbed energy E in the BW denominators. Note that the "hole" lines in these BW diagrams have only a single segment. There are no interactions attached to the middle of these lines.

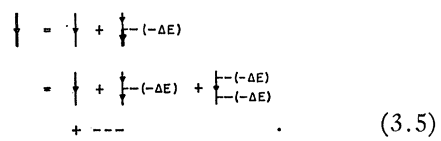
The first step in obtaining the usual RS perturbation series is to iterate the identity connecting the BW and RS denominators,

$$(E-E_i)^{-1}$$
$$=(E_0-E_i)^{-1}+(E_0-E_i)^{-1}(-\Delta E)(E-E_i)^{-1}. \quad (3.3)$$

This can be expressed in operator language,

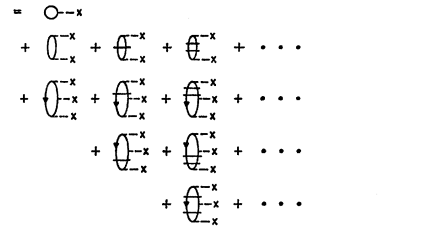
$$e_{BW}{}^{-1}=e_{RS}{}^{-1}+e_{RS}{}^{-1}(-\Delta E)e_{BW}{}^{-1} \quad (3.4)$$

and also graphically:



(3.5)

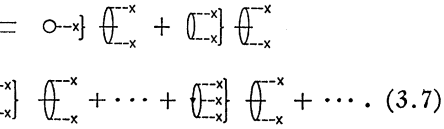
The $(-\Delta E)$ insertions belong not only to the downgoing line, but to the *entire* intermediate state. It will be more convenient to represent these by horizontal bars cutting across the entire diagram at the appropriate levels. The expansion for ΔE can therefore be expressed as



(3.6)

The plain hole line now indicates the use of RS denominators, and each horizontal bar stands for an insertion of $(-\Delta E)$.

We now have an expansion for ΔE in terms of ΔE, so one can iterate this by inserting the expansion back into itself. For example,

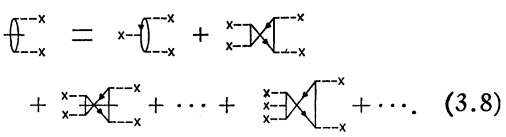


(3.7)

Each horizontal bar accompanied by a bracket indicates that (minus) a term of the series (3.6) is to be

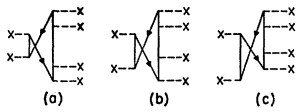
[57] This idea is implicit in all attempts to calculate the Brueckner reaction matrix in finite nuclei. See especially Refs. 2, 8, 10, 12, and 24.

inserted in place of $(-\Delta E)$ at the level of that bar. These diagrams can be drawn more compactly by "exchanging" the hole lines of the original diagram and the inserted diagram to form a "single-loop" diagram. Thus (3.7) is replaced by



(3.8)

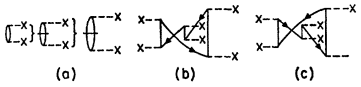
One can keep track of the minus signs [originating from the $(-\Delta E)$'s] by including a factor of $(-1)^{l+h+b}$, where l is the number of closed loops, h the number of hole-line segments (counted without regard to any remaining horizontal bars), and b is the number of brackets remaining (in cases where the hole–line exchanges have not been carried out everywhere). In this form, the rule applies to both (3.7) and (3.8). In both cases a horizontal bar *without* a bracket still stands for $(-\Delta E)$. All interactions within the insertion part of a (3.8)-type diagram must be kept within the vertical limits defined by the original RS denominator in which this insertion is placed. Thus (a) of (3.9) is allowed, while (b) and (c) are not.



(3.9)

One must also be careful to associate the correct RS denominators with these diagrams. For the levels *within* an insertion, one must use the RS denominators appropriate for the inserted part alone. In other words, the insertions are to be evaluated "on the energy shell."

One can repeat this procedure and insert the expansion back into itself any number of times. The RS expansion, up to any desired order, is generated by repeating this process until $(-\Delta E)$'s no longer appear in diagrams up to that order. There is an ambiguity, however, in the placement of insertions in second and higher "generations" of graphs. For example, one wonders which of the forms (b), (c) of (3.10) to use to indicate the sequence of insertions shown in (a). These two forms are equivalent, according to the discussion so far.



(3.10)

Later developments will be simplified if we choose form (b), or in general if we always place nth generation insertions in the hole lines connected to the *bottoms* of the $(n-1)$th generation insertions. Then there is no such diagram as (c) of (3.10) in the RS perturbation series.

We now observe that the single-loop graphs, such as (b) of (3.10), resemble certain of the Goldstone diagrams for a single particle in an external field. Let us write the Hamiltonian in "second-quantized" form,

$$H=\sum_i E_i\eta_i^\dagger\eta_i+\sum_{ij}V_{ij}\eta_i^\dagger\eta_j, \tag{3.11}$$

and draw all the diagrams which occur when this is used in a Goldstone expansion. One finds all the diagrams of RS form, as described above, and many more, including such terms as (b) and (c) of (3.9) and (c) of (3.10). But there is also a difference in the definition of the energy denominators. The Goldstone denominators are given by the sum of *all* downgoing line energies minus the sum of *all* upgoing line energies. In other words, the insertions are now evaluated "off the energy shell."

These expansions for ΔE must be equivalent. The connection is established by showing that the Goldstone graphs may be arranged in groups such that each group is equivalent to an RS graph. To see which Goldstone graphs correspond to a given RS graph, take the RS graph and relax the "time" restrictions [discussed in connection with (3.9)] placed on the interactions of the inserted parts *with respect to the remainder of the diagram*, subject to the following condition. The *top* interaction of each inserted part, i.e., the top of each series of upgoing line segments, is to be kept in its original position *with respect to the part of the diagram in which it was originally inserted.* In other words, the top of an nth generation insertion is to be held fixed with respect to the $(n-1)$th generation insertion in which it was placed. The remaining interactions in this insertion (and in "higher generation" insertions within this, subject ot the same condition) can be freely displaced in the downward direction. The equivalent Goldstone graphs are all those which are generated by this procedure. One can also apply this rule in reverse, to uniquely associate each Goldstone graph with a certain RS graph, and thus with a definite sequence of insertions from the iteration of (3.6). This is the point where it is useful to have chosen form (b) over form (c) in (3.10). Thus, (c) of (3.10) now corresponds to two "first-generation insertions.

This equivalence follows from an algebraic identity between the products of the energy denominators. This is the same identity which permits unlinked diagrams to be factored in Goldstone's time-dependent formalism, and also in the analogous "temperature-dependent" methods of quantum statistics. In these examples, the factorization comes about when the time (temperature) ordering of the interactions is generalized by the mathematical device of redefining some of the limits of integration in the multiple time (temperature) integrals. It is not so widely recognized that this identity also applies, in certain cases, to various parts of a single linked diagram. This has been emphasized especially by Bethe, Brandow, and Petschek.[48] A purely algebraic proof of this "factorization theorem" has been given by Frantz and Mills.[27] But the algebraic

proof is rather cumbersome, especially when there are several linked parts (or insertions) to be factored (or placed on the energy shell) simultaneously. The result is much easier to visualize when some sort of a multiple integral is used. BBP[48] based their discussion on the adiabatic time integrals used by Goldstone, although temperature integrals would have served just as well. For the present it is simplest, since we need not attribute any physical significance to the variables of integration, to represent the energy denominator products by integrals of the form

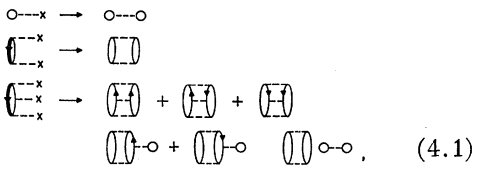
$$(-1)^n \int_{-\infty}^{0} d\tau_n \int_{-\infty}^{\tau_n} d\tau_{n-1} \cdots \int_{-\infty}^{\tau_2} d\tau_1 \exp\{\sum_{j=1}^{n} \tau_j \delta E_j\}. \tag{3.12}$$

Each δE_j is the *change* in the intermediate state energy caused by the jth interaction. To obtain the energy factor for a particular Goldstone diagram, or for the complete set of these which is equivalent to an RS diagram, the rule is to arrange the limits of integration so that the order of the τ_j's is restricted in just the same way as the order of the interactions they represent. The integrals are easily evaluated, and the theorem follows immediately. (An example is worked out in detail in BBP.)

This factorization theorem is the only feature of our linked-cluster derivation (apart from the use of second quantization,[58] and diagrams) which might be considered nonelementary. This is the general form of the identity which Brueckner used in his original study of linked clusters,[25,26] and it occurs in one form or another in most of the derivations which have appeared since then. For example, it seems quite natural that Hugenholtz[29] used convolution integrals to unlink his diagrams, since his derivation is essentially the Fourier transform of Goldstone's multiple-integral method.

IV. THE GOLDSTONE EXPANSION

Much of the preceding discussion also applies to a nondegenerate N-body system, since *any* perturbation problem is, through (3.11), formally equivalent to the problem of a single particle in an external field. Thus one can identify each "one-body" state Φ_i with an N-body Slater determinant. Each of the "one-body" BW graphs of (3.2) can be directly translated into a set of N-body graphs. For example,



(4.1)

plus exchange diagrams, plus diagrams with "momentum-nonconserving" terms which change a particle into a hole (or vice versa), plus diagrams containing the negative of any one-body "model" potential which may have been included in H_0.

If one thinks of Slater determinants, some of the summations over particle and hole states must be restricted to avoid "exclusion-violating" terms. It is much simpler to use the machinery of second quantization[58] (which is guaranteed to preserve antisymmetry), for then one need never mention exclusion except to distinguish between "particle" and "hole" states. This treatment, based on

$$H_0 = T + V_{\mathrm{SM}} = \sum_i E_i \eta_i^\dagger \eta_i$$

$$V = v - V_{\mathrm{SM}}$$

$$= \tfrac{1}{2} \sum_{ijkl} \langle ij \mid v \mid kl \rangle \eta_i^\dagger \eta_j^\dagger \eta_l \eta_k - \sum_{ij} \langle i \mid V_{\mathrm{SM}} \mid j \rangle \eta_i^\dagger \eta_j, \tag{4.2}$$

(where V_{SM} is a "shell-model" potential, not necessarily self-consistent), shows that it is quite proper to sum each particle or hole line over *all* such states, regardless of exclusion. From this viewpoint, the exclusion principle is simply a statement concerning the pairwise cancellation of certain terms belonging to different diagrams. The algebra of the Fermion operators then leads to the diagram rules, as discussed for example in Appendix B.

Diagram Analysis

In general, each diagram consists of a number of *linked parts* which are not connected to each other in any way, as in the last of the diagrams shown above. These linked parts must all overlap in such a way that gaps representing the initial or "vacuum" state Φ_0 do not appear anywhere between the top and bottom of the entire diagram. Since these are Brillouin–Wigner diagrams, their energy denominators are given by

$$e_{\mathrm{BW}} = E - H_0 = E_0 + \Delta E - H_0. \tag{4.3}$$

We now expand out ΔE *just once*, as in (3.3) to (3.6). The most general diagram now consists of a group of overlapping linked parts, with RS denominators

$$e_{\mathrm{RS}} = E_0 - H_0, \tag{4.4}$$

and with a number of horizontal bars indicating $(-\Delta E)$

[58] The formalism of second quantization is, of course, completely equivalent to the use of Slater determinants. For a very thorough discussion, see S. Schweber, *An Introduction to Relativistic Quantum Field Theory* (Harper and Row, New York, 1961). For a straightforward and elementary derivation of this formalism, starting from Slater determinants, see F. Villars, Ref. 20. A very clear and elegant derivation of this type has been given by G. Wick (unpublished lecture notes). A condensed form of the latter is available in the book by G. E. Brown, Ref. 18.

insertions. Note that if we translate the first "one-body" graph appearing on the right side of (3.7) into an N-body graph, we obtain an *unlinked* graph which, except for a minus sign, is just the same as the last diagram shown in (4.1). In other words, the unlinked diagram is cancelled by a term from the expansion of the $(-\Delta E)$ insertion. This sort of cancellation was confirmed by Brueckner[25,26] up to at least sixth order. We shall now demonstrate that it occurs to all orders.

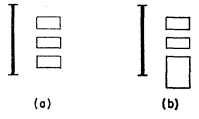
The first step is to introduce some definitions:

(i) The *principal part* of a diagram is that linked part which contains the topmost interaction of the entire diagram. It does *not* include any $(-\Delta E)$ insertions.

(ii) An *overlapping group* consists of a group of $n \geq 1$ linked parts which overlap each other, such that the whole group contains no gaps representing the "vacuum" state Φ_0 as an intermediate state. All $(-\Delta E)$ insertions occurring within the "time limits" (i.e., between the bottommost and the topmost interactions) of the group are to be included.

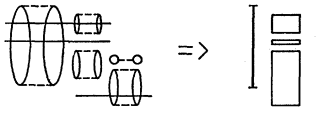
(iii) A *time block* can consist either of an overlapping group (which may contain ΔE insertions) or of an isolated $(-\Delta E)$ insertion.

According to these definitions, removal of the principal part from an arbitrary diagram (think of simply erasing this part of the diagram) will leave a number (≥ 0) of time blocks. The latter will be separated vertically by gaps corresponding to the vacuum state. This structure is shown schematically in (4.5), where the long vertical bar represents the principal part, and the rectangles indicate time blocks.



(4.5)

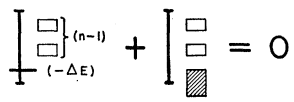
The bottom of the lowest time block may occur above the bottom of the principal part, as in (a), or, if this is an overlapping group (in contrast to a ΔE insertion), its bottom interaction may also occur below the principal part, as in (b). The analysis of a typical diagram is shown in (4.6).



(4.6)

Consider a diagram with $n \geq 1$ time blocks (counted as if the principal part had been removed), where the lowest of these is a $(-\Delta E)$ insertion. Expand out this insertion in terms of a series of inserted diagrams, as indicated in (3.7). These inserted parts are all "on the energy shell" at this stage, meaning that their RS energy denominators are unaffected by the original diagram in which they were inserted. Now the factorization theorem can be used to show that each of these (3.7)-type diagrams is equivalent to a set of diagrams with Goldstone energy denominators, i.e., denominators determined by both the inserted and original parts. Each inserted part (itself an overlapping group) is allowed to take on all relative positions with respect to the original part (the principal part), except for one restriction. The topmost interaction of the inserted part must always occur at the same level of the original diagram as the $(-\Delta E)$ which it arose from.

Except for a minus sign from $(-\Delta E)$, this procedure generates all of the diagrams whose principal part and topmost $(n-1)$ time blocks coincide with the original diagram, and which contain an overlapping group extending downwards from the level where the $(-\Delta E)$ was. This result is shown schematically as



(4.7)

where the shaded rectangle represents all possible overlapping groups extending downwards from the $(-\Delta E)$ level. Finally, we note that every N-body diagram of type (4.5) is either just a principal part, or else it fits into one of the categories (a), (b) of (4.7). (Remember that the unshaded blocks can represent $(-\Delta E)$ insertions, as well as overlapping groups.) This shows that all diagrams cancel, and may therefore be ignored, *except for the principal parts*. This is just Goldstone's result.

Note that this argument focusses directly on the elimination of unlinked terms, bypassing most of the diagram rules. It remains valid when a one-body interaction, $-V_{\mathrm{SM}}$, is included. It would also apply equally well to systems with n-body interactions, $n > 2$.

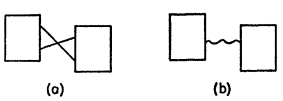
Rates of Convergence, Generalized Time Ordering

It is obvious, physically, that $\Delta E \propto N$ for a large saturating system. If one could ignore the effect of the large shifts ΔE in the energy denominators, each linked part of a general diagram would contribute a factor proportional to N. (This is demonstrated in Appendix C.) A general nth-order BW graph, with $n-1$ energy denominators and L linked parts, is therefore proportional to N^{L+1-n}. But $n \geq L+1$, except for the lowest-order $(n=1,\ L=1)$ diagram, so the $(\Delta E/N)$ contributions from all except the first of the BW diagrams are of order N^{-1} or less. Brueckner[25,26] has drawn attention to this "fictitious convergence" of the BW expansion, as well as the "fictitious divergence" of the RS series due to unlinked terms of order N^L. But, as Brueckner first observed, in each order of the RS expansion the unlinked terms must all cancel. This leaves a "linked RS expansion" in which each term is clearly of order N.

One might now ask whether such a "linked RS expansion," as discussed by Brueckner, is identical to the Goldstone expansion. The answer depends on the treatment of the so-called "exclusion-violating" (e.v.) terms. The distinction emerges most clearly when one begins by *consistently omitting* all e.v. terms. (It is consistent, in the original BW expansion, to either include or omit all the e.v. terms. Omission means that each BW intermediate state corresponds to an actual Slater determinant.) The expansion (3.7) of $(-\Delta E)$ then generates both e.v. and non-e.v. terms. To cancel the unlinked terms of the original BW expansion, as in (4.7), one need only apply the factorization theorem to the non-e.v. terms. The e.v. terms, which remain unlinked and "on the energy shell," can then be converted into linked diagrams by "exchanging" a pair of lines as in (3.8). The resulting linked RS expansion is not quite the same as the Goldstone expansion. In fact, this expansion should converge somewhat faster than Goldstone's. The latter is obtained by using the factorization theorem to take these e.v. insertions off the energy shell, and this necessarily increases the number of terms in the expansion.

This brings us to the important point that many Goldstone diagrams contain both e.v. and non-e.v. terms in their summations over single-particle states. [Consider diagram (4.8a) for a finite system lacking momentum conservation.] These non-e.v. terms can *also* be put on the energy shell, since the applicability of the factorization theorem depends only on the diagram's topology. It turns out that there are also *other* parts of linked diagrams which can be similarly converted into on-energy shell insertions. The basic criterion[48] is that the topological structure must permit the "time order" of one subset of interactions to be generalized with respect to the remaining interactions, in an unrestricted manner in one direction (either downwards or upwards), without altering any of the single-particle state labels. When the factorization theorem is used this way, to partially sum certain classes of Goldstone diagrams, we shall call this the g.t.o. (generalized time order) treatment, and the resulting diagrams g.t.o. diagrams. This treatment has been shown to greatly improve the *practical* rate of convergence of the series.[9]

Two classes of diagrams deserve special mention as candidates for this g.t.o. treatment. (Their practical importance is discussed in Sec. IX.) One consists of all diagrams arising from the e.v. terms discussed above. These always consist of two "almost separate" parts joined together by two crossed lines (or four, or any even number), as indicated in (4.8a).



(4.8)

Another important class involves two "almost separate" parts joined by a single interaction (potential or reaction matrix), as shown in (4.8b). Note that this g.t.o. treatment allows reaction matrices to be evaluated on the energy shell, if and only if this treatment applies *separately* to each of the v-interaction ladders contained in the reaction-matrix elements.

The present derivation puts the problem of strict mathematical convergence in a particularly bad light. The initial step, expanding ΔE out of the BW energy denominators, cannot be rigorously justified unless the smallest unperturbed energy difference (E_1-E_0), which is of order $N^{-1/3}$ in large nondegenerate systems, is larger than ΔE. This suggests a radius of convergence of order $N^{-4/3}$. The actual radius could conceivably be much larger than this, thanks to having eliminated the large number of unlinked terms. For example, Baker[59] has given a physical argument that this radius should scale only as $N^{-\gamma}$, with $\frac{1}{3}\leq\gamma\leq 1$. But this is not much consolation—the expansion must still be an asymptotic one. (The g.t.o. treatment cannot alter this situation, which is due only to the large number of particles.) Katz[60] and Baker[59] have shown, however, that in certain cases the linked-cluster expansion represents a satisfactory analytic continuation. We return to this discussion in Sec. IX.

V. THE BLOCH–HOROWITZ EXPANSION

The degenerate formalism of Sec. II, i.e. (2.14), is quite general. All it requires is that E be removed from all "nondegenerate" E_i's by a finite amount, so that the operators are all well-defined. It can therefore be used when H_0 is a shell-model Hamiltonian and the Φ_i's are N-body Slater determinants. What Bloch and Horowitz[44], and Day[45] have done is to obtain a linked-cluster expansion for the matrix elements of $\mathcal{U}$, in terms of the "true" two-body interaction v. This can be partially summed to give an expansion in two-body reaction matrices, just as in the Goldstone case.

These authors begin with an H_0 for which the single-particle energies are assumed to exhibit some sort of discrete shell structure, at least for the low-lying states. They divide the single-particle states into three categories, which we shall call core, valence, and intermediate states, and which we denote, respectively, by l, m, n, etc.; λ, μ, ν, etc.; and a, b, c, etc. The quasi-degenerate subspace D (the model subspace) consists of all $(N+n)$-body determinants defined as follows. N is the number of core states, and these are always occupied by the N core particles. The remaining n valence particles must then be distributed among the available valence states. The valence-state energies E_μ need not be strictly degenerate, and collective phenomena can be studied by including more than one shell in the definition of these states.

[59] G. A. Baker, Phys. Rev. **131**, 1869 (1963).
[60] A. Katz, Nucl. Phys. **20**, 663 (1960); also in *Lectures on the Many-Body Problem* (Bergen, 1961), C. Fronsdal, Ed. (W. A. Benjamin, Inc., New York, 1962).

Let us left-multiply (2.14) by $\mathbf{A}^\dagger$, and express the result as

$$\Delta E = E - E_0 = \mathbf{A}^\dagger \mathcal{U} \mathbf{A}, \tag{5.1}$$

where

$$E_0 = \mathbf{A}^\dagger H_0 \mathbf{A} = E_{0C} + E_{0V}, \tag{5.2}$$

$$E_{0C} = \mathbf{A}^\dagger H_{0C} \mathbf{A} = \sum_m^N E_m, \tag{5.3}$$

$$E_{0V} = \mathbf{A}^\dagger H_{0V} \mathbf{A} = \sum_\mu E_\mu P_\mu^{(0)}, \tag{5.4}$$

$$H_{0C} = \sum_m^N E_m \eta_m^\dagger \eta_m, \tag{5.5}$$

$$H_{0V} = \sum_\mu E_\mu \eta_\mu^\dagger \eta_\mu. \tag{5.6}$$

(We assume that $\mathbf{A}^\dagger \mathbf{A} \equiv \langle \Psi_D \mid \Psi_D \rangle = 1$.) The *model* probability of state μ being occupied is

$$P_\mu^{(0)} = \langle \Psi_D \mid \eta_\mu^\dagger \eta_\mu \mid \Psi_D \rangle = \sum_{j(\mu)} \mid a_j \mid^2, \tag{5.7}$$

where $j(\mu)$ includes all determinants Φ_j, $j \in D$, in which state μ is occupied. Note that (5.1) is formally very similar to (3.1), except that $\mathcal{U}$ and H_0 are now $d \times d$ matrices.

Diagonal Transformation

General properties of the solution can be used to simplify the $\mathcal{U}$ matrix. This matrix is Hermitian when the E appearing in the Green's function (2.7) is taken to be a fixed parameter. In principle, therefore, one can determine $\mathcal{U}(E_\alpha)$, where E_α is the desired eigenvalue, and solve

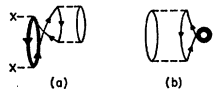
$$[H_0 + \mathcal{U}(E_\alpha) - E_\beta^{(\alpha)} \mathbf{I}] \mathbf{A}_\beta^{(\alpha)} = 0 \tag{5.8}$$

to obtain *d orthogonal* $\mathbf{A}_\beta^{(\alpha)}$'s. (Generally speaking, only $\mathbf{A}_\alpha^{(\alpha)} = \mathbf{A}_\alpha$ and $E_\alpha^{(\alpha)} = E_\alpha$ will be physically significant.) These $\mathbf{A}_\beta^{(\alpha)}$'s will now be used to define a new basis for the degenerate subspace. In the case of exact degeneracy (all E_μ's equal to $\bar{E}_\mu$, $E_{0V} \rightarrow n\bar{E}_\mu$, $H_0 \rightarrow E_0 \mathbf{I}$), H_0 will remain diagonal under this transformation, therefore $\mathcal{U}$ itself will be diagonalized. This is very convenient, so we shall assume strict degeneracy for now. This restriction will be removed later on.

Diagram Analysis, Core and Valence Energies

The analogy between (5.1) and (3.1) is much clearer in this new representation, because (5.1) now involves only the single matrix element $\mathcal{U}_{\alpha\alpha}$. This element can be obtained, formally, by iterating (2.12). The various terms in the expansion of (5.1) can thus be represented by means of "one-body" BW diagrams which look exactly like those in (3.2). The heavy downgoing line now refers to the desired "shell-model" state $\mathbf{A}_\alpha^{(\alpha)} = \mathbf{A}_\alpha$, with energy E_α, and the states described by the upgoing line segments are all of the Φ_i's for $i \notin D$. The $\mathbf{A}_\beta^{(\alpha)}$'s are all excluded by the projection operator Q in (2.7).

These "one-body" BW diagrams can now be translated into "$(N+1)$-body" diagrams in which the N core particles are described by the familiar Goldstone convention, the N-body "vacuum" representing the fully occupied core. The n valence particles may, for the present, be indicated simply by a single heavy line. The "vacuum state" for these valence particles indicates that they are distributed as in the shell-model state $\mathbf{A}_\alpha$. An upgoing valence line segment must carry labels indicating the single-particle states occupied by *each* of these n particles. (With this convention, interactions among these valence particles must be illustrated as interactions with a fictitious external potential. It would be more explicit to replace each valence line by n separate lines, but this is not essential for the present task of eliminating unlinked diagrams.) Note that each *downgoing* valence line consists of only a single segment, just as in the diagrams of (3.2). The "core-valence exchange" terms, which occur when a valence particle and a core particle both happen to be in the same single-particle state, can be illustrated as in the following examples.

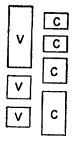


(5.9)

The most general BW diagram is of unlinked form at this stage, consisting of a number of separate linked parts which all overlap vertically such that the vacuum or shell-model state $\mathbf{A}_\alpha$ does not appear anywhere as an intermediate state. The linked parts fall into two categories. The *core parts* are those in which there are no interactions involving any of the particles which originally come from valence states. [Note, however, that this definition allows core particles to scatter *into* valence states. Any resulting terms which violate exclusion are compensated by "core–valence exchange" terms like those of (5.9). The core parts are *exactly* the same as the linked parts for the closed-shell nucleus that one would obtain by *physically removing* the valence particles.] All other linked parts, including exchange terms such as (5.9), are called *valence parts*. These may involve core particles as well as valence particles.

Now imagine a typical unlinked BW diagram from which all the linked core parts have been temporarily removed. The remaining diagram will generally consist of a number of overlapping groups, each of which contains one or more linked valence parts. These overlapping *valence groups* are separated vertically by gaps which, in the absence of the core parts, correspond to the vacuum state $\mathbf{A}_\alpha$. Overlapping *core groups* are defined similarly, by temporarily removing the linked valence parts. An unlinked BW diagram may thus be analyzed into several overlapping groups of each variety, the groups of one variety covering the gaps between those of the other variety. An example of this

overlapping group structure is shown schematically in (5.10).



(5.10)

Core and valence interaction energies, ΔE_C and ΔE_V, are defined below such that

$$\Delta E=\Delta E_C+\Delta E_V. \tag{5.11}$$

The BW denominators can therefore be expressed as $e_{\mathrm{BW}}=E_0+\Delta E_C+\Delta E_V-H_0$. We remove ΔE_C from *every* denominator, using the expansion technique of (3.3) to (3.6). The ΔE_V's are similarly removed, but *only* from those denominators which do not involve any valence parts, e.g., from the denominators which belong to gaps between the valence parts. "Time blocks" are now introduced as follows. A *core block* can be either an overlapping core group, *including* any $(-\Delta E_C)$ insertions within its vertical limits, or it can be a single $(-\Delta E_C)$ insertion which only cuts through valence parts. A *valence block* can be either a valence group, *not* including any $(-\Delta E_C)$ insertions, or it can be a single $(-\Delta E_V)$ insertion. The core interaction energy ΔE_C can now be defined. This is taken to be the sum of all diagrams consisting of only a single core block. Note that (5.11) then specifies ΔE_V. The time-block structure of a complete diagram follows the same general pattern as its overlapping group structure, except that ΔE_C and ΔE_V insertions will often make the number of time blocks larger than the number of overlapping groups. This time-block structure can also be represented by diagrams like (5.10).

Consider a diagram whose *lowest two* time blocks consist of a valence group and a $(-\Delta E_C)$ insertion within this. As in the Goldstone expansion, this cancels all diagrams which are identical except for this lowest $(-\Delta E_C)$ being replaced by some other kind of core block whose topmost interaction occurs at the same level where this $(-\Delta E_C)$ was. Let us now assume the answer we wish to obtain, namely, that ΔE_V is given by the sum of all diagrams consisting of just a single valence group. A similar phenomenon then occurs when the lowest two time blocks are a core group and a $(-\Delta E_V)$ insertion. This argument demonstrates that *all diagrams with more than one time block may be ignored.* The sum of all single-core-block diagrams is ΔE_C, by definition, and we have already seen (Sec. IV) that this is equal to just the sum of all *linked* core parts. This is simply the Goldstone prescription for the interaction energy of the closed-shell nucleus obtained by *physically removing* all the valence particles. The sum of the remaining diagrams must, according to (5.11), be ΔE_V. But these are just the diagrams assumed above. This confirms that the assumed form of ΔE_V is indeed a consistent solution.

Shell-Model Secular Equation

The ΔE_C part of the calculation is clearly quite independent of $\mathbf{A}_\alpha$ and ΔE_V. That is, ΔE_C must be the same for *all* of the degenerate eigenstates $\mathbf{A}_\alpha$. This implies that the $\mathfrak{V}$ matrix must have the form

$$\mathfrak{V}=\Delta E_C\mathbf{I}+\mathfrak{V}_V, \tag{5.12}$$

where $\mathfrak{V}_V$ is given by the sum of all valence groups. This result is very convenient, because (5.2) to (5.6) can then be used to reduce the original secular equation, (2.14), to the much simpler "shell-model" form

$$[H_{0V}+\mathfrak{V}_V(E_V)-E_V\mathbf{I}]\mathbf{A}=0. \tag{5.13}$$

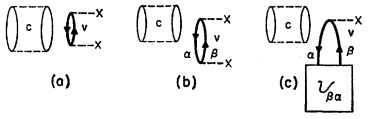
All "core" quantities have been eliminated from this expression. The valence Hamiltonian, H_{0V}, is just the projection [see (5.6)] of H_0 onto the valence states μ, and the *total valence energy*, $E_V=E_{0V}+\Delta E_V$, is the total energy E minus the *total core energy*, $E_C=E_{0C}+\Delta E_C$. (This E_C represents the total energy of the closed-shell nucleus obtained by physically removing the valence particles.[45]) We note, finally, that the denominators in the expansion of $\mathfrak{V}_V$ are given by

$$e_V=e_{\mathrm{BW}}-\Delta E_C=E_V+E_{0C}-H_0, \tag{5.14}$$

so $\mathfrak{V}_V$ depends on the *total* valence energy E_V. (The E_{0V} part of this E_V dependence is nontrivial, in the quasi-degenerate case, since E_{0V} then depends on the model state $\mathbf{A}_\alpha$.)

Spurious Terms

An important part of this derivation has not been mentioned yet. Consider the upgoing valence line in (a) of (5.15).



(5.15)

This line can describe a situation where all the valence particles remain in valence states, but with a different arrangement than in the model state $\mathbf{A}_\alpha{}^{(\alpha)}$. This possibility is not excluded by the Q operator in (2.7), thanks to the core excitation occurring at the same level, so this term must be included in the expansion. But a truly degenerate intermediate state $\mathbf{A}_\beta{}^{(\alpha)}$ would occur if this valence-particle arrangement were permitted in diagram (b). This poses a problem, because the cancellation argument requires that the set of allowed states within an overlapping group be independent of the rest of the diagram.

One can get around this dilemma by the following device.[61] We shall always allow the upgoing valence lines to describe *all* possible arrangements of these particles, except for the initial $\mathbf{A}_\alpha{}^{(\alpha)}$ arrangement,

[61] This argument has also been used by Dawson, Talmi, and Walecka, Ref. 17.

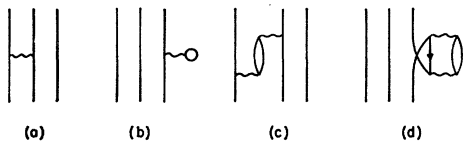
regardless of whether core excitations are present or not. This amounts to treating the states $\mathbf{A}_\beta^{(\alpha)}$, $\beta \neq \alpha$, as valid intermediate states. This device treats diagram (a) correctly, but it includes some spurious terms in (b). (The denominators contain ΔE_V, so these terms remain well-defined. These spurious terms will not appear in the final result, therefore they should not affect its convergence.) Let us now group a spurious term from diagram (b) together with *all other* spurious terms obtained by replacing the bottom interaction by all possible sequences of interactions leading to the same spurious state $\mathbf{A}_\beta^{(\alpha)}$. We observe that the sum of all such terms is equivalent to diagram (c), where the spurious state β is created from the vacuum state α by the matrix element $\mathcal{U}_{\beta\alpha}(E_\alpha)$. But this element must be zero, since it is off-diagonal in a representation chosen to diagonalize $\mathcal{U}$. [Actually, the $\mathcal{U}_{\beta\alpha}$ element in (c) should be replaced by an infinite "geometric" series,

$$\mathcal{U}_{\beta\alpha}+[\mathcal{U}(P'/e_V)\mathcal{U}]_{\beta\alpha}+[\mathcal{U}(P'/e_V)\mathcal{U}(P'/e_V)\mathcal{U}]_{\beta\alpha}+\cdots,$$

P' being the projection operator onto all of the $\mathbf{A}_\beta^{(\alpha)}$'s except $\mathbf{A}_\alpha^{(\alpha)}$, but this does not affect the result.] Thus one finds that *all* spurious terms cancel, so no harm is done by including them. After demonstrating the cancellation of all diagrams with more than one group, one may then remove these spurious terms by the same argument.

Our derivation of the Bloch–Horowitz expansion is now essentially complete. All that remains is to return from the $\mathbf{A}_\beta^{(\alpha)}$ representation to the Φ_i representation (where the valence-state occupation numbers are all 1 or 0), and to express the i, j elements of $\mathcal{U}_V$ in terms of diagrams with n upgoing external lines. Each group of external lines, at the top and bottom of a BH diagram, must be labelled with n *distinct* valence states. Further details of these diagrams are discussed in Appendix B. Finally, upgoing "ladders" of two-body interactions can be grouped together to form an expansion in two-body reaction matrices, just as in the Goldstone case.

Some simple valence diagrams are shown in (5.16), for the case $n=3$.



(5.16)

Diagram (a) demonstrates that the leading term in the effective two-body interaction is the Brueckner reaction matrix, as has been known for many years.[46,47,17] Diagram (b) is the corresponding "Hartree–Fock" contribution[2–4,9] to the shell-model potential acting on the valence particles. Diagram (c) is a correction to (a) arising from core polarization. It can be regarded as the exchange of a virtual core phonon. This illustrates the fact that the reduced secular equation (5.13) has only eliminated the *static* features of the core. All *dynamical* core effects are included in the valence interaction $\mathcal{U}_V$.

Diagram (d) represents a *change* in the core interaction energy due to the "blocking" (exclusion) effect of the valence particles. This is one of the core-valence exchange diagrams that were first encountered in (5.9). It is convenient to absorb this term into the definition of the valence particle V_{SM}, in addition to term (b). We emphasize again that $\mathcal{U}_V$ contains *all* effects due to the physical addition of the valence particles, both the "new" processes discussed above, and all of the *changes* in the "old" core-correlation processes.

Quasi-Degeneracy

The assumption of exact degeneracy was needed to ensure that $\mathcal{U}(E_\alpha)$ be diagonal in the $\mathbf{A}_\beta^{(\alpha)}$ representation defined by $H_0+\mathcal{U}(E_\alpha)$. Suppose now that a one-body "potential" with the simple form

$$V_1=\sum_\mu (E_\mu-\bar{E}_\mu)\eta_\mu^\dagger\eta_\mu \qquad (5.17)$$

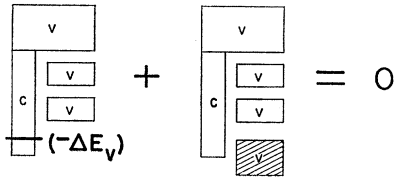
is added to V. ($\bar{E}_\mu$ is the degenerate valence state energy.) A simple inspection of the BH diagrams shows that the result of using $V+V_1$ in (5.13) is exactly the same as if one had included V_1 in H_0 (instead of in V) without regard to the niceties of the derivation. Thus exact degeneracy is not necessary in practice.

Reduced BH Expansion

The present derivation suggests a way to simplify the BH expansion. It was shown above that $\mathcal{U}_V$ is given by the sum of all valence *groups*, meaning that a typical diagram may contain several overlapping valence parts. (We refer again to the $\mathbf{A}_\beta^{(\alpha)}$ representation and the "valence vacuum" convention.) Each valence part may have several sections of valence particle excitations, separated vertically by sections with nothing but core excitations. An example is the right-hand valence part in (5.20a), which is our schematic representation of (5.21a). As illustrated in this example, there may also be *projecting core excitations*, which extend vertically beyond the topmost or the bottommost valence interaction of that part. (*Valence interactions* are interactions involving any of the original valence particles, regardless of whether these happen to be in valence states at the time of interaction.) Reference to the original BW expansion of $\mathcal{U}$ shows that a valence excitation (or a passive valence interaction) can be overlapped *only* by one or more core excitations (which may or may not be "projecting"). Valence excitations in separate valence parts cannot overlap each other, or overlap passive valence interactions, because at any given level there can be no more than one downgoing and one upgoing (n-body) valence line.

It frequently happens that a valence group has the form of several separate valence groups which overlap

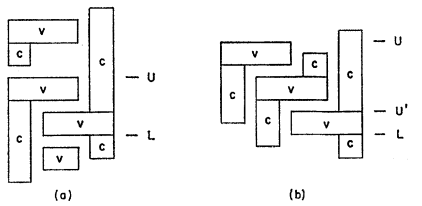
only because of a projecting core excitation extending downwards below the lowest valence interaction in the topmost group. All of these valence groups, except the topmost one, may be discarded if we simultaneously remove ΔE_V from the denominators in the projecting core excitation. This cancellation is shown schematically in (5.18), where the unshaded lower rectangles represent valence blocks (valence groups or ΔE_V insertions), and the shaded rectangle indicates the sum of all valence groups extending downwards from the ΔE_V level.



(5.18)

Core excitations projecting *above* a valence group can be treated similarly, because the factorization theorem (a purely algebraic identity) works "upwards" as well as "downwards." Finally, one is left with only the "irreducible" valence groups, provided that core-type denominators (5.22) are used within all projecting core excitations. *Irreducible valence groups* are those which contain no valence parts that overlap *only* by virtue of *projecting* core excitations.

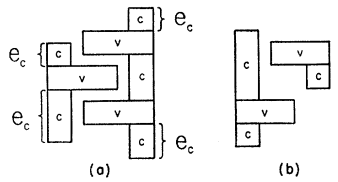
A little more care is needed to complete this argument. Consider the diagram (5.19a).



(5.19)

Examine all the *downward* projecting core excitations (p.c.e.'s), and identify the level "L" below which these p.c.e.'s become "properly projecting," meaning that the valence parts below this level (if any) are joined to the rest of the diagram *only* by virtue of their being overlapped by these p.c.e.'s. Now expand ΔE_V out of all denominators *below* this level L, and apply (5.18). Similarly, identify the level "U" above which all the *upward* p.c.e.'s become "proper", and apply the cancellation argument above this level. There remains the problem of diagrams, like that in (5.19b), which overlap "both ways." At this stage the *downwards* p.c.e.'s can all be completely factorized by means of (3.12), by associating an additional excitation energy ΔE_V with the δE_j of the valence interaction at level L. One may therefore "erase" all the downwards p.c.e.'s, and replace them by numerical factors multiplying the appropriate valence parts. The upwards p.c.e.'s then become proper at the new level U', and the reduction is easily completed.

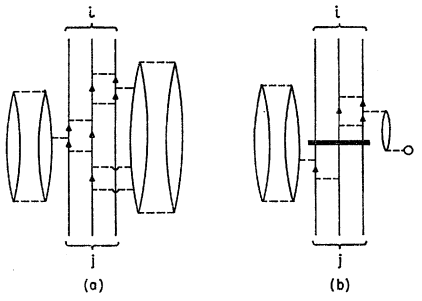
We now give some examples to illustrate this result. The two valence parts shown in (5.20) (a) form an irreducible valence group, while those in (b) are obviously reducible.



(5.20)

In (a), the middle valence excitation is "trapped" between the other valence excitations. This prevents the factorization theorem from being applied, either upwards or downwards, to place the left-hand valence excitation on the energy shell. The factorization theorem *can* be used, however, to put all the projecting core excitations on the energy shell. The locations of these on-energy-shell core denominators e_C are shown in the figure.

Coming back to the Φ_i representation and to diagrams with n external lines, we find that the above definition of irreducible diagrams is still easy to apply. Examples of diagrams like (5.20) are shown in (5.21),



, (5.21)

where the upgoing arrows indicate valence particles excited to intermediate states. For these "external-line" graphs, however, one is tempted to use another definition of reducibility: If it is possible to obtain two valence diagrams from one, simply by cutting *all* n of the valence lines at some level and then separating the top and bottom parts, the original diagram is reducible. The heavy line in (5.21b) indicates where this diagram may be cut in two. Unfortunately, this "field-theoretic" definition is too general, since it also includes cases where overlaps result from "projecting valence excitations" whose structure resembles (5.16d). These cases require a separate treatment, which we shall not discuss here. [See, however, the discussion below (8.24).]

This reducibility argument has assumed exact degeneracy among the valence states, but again this restriction is easily removed by means of (5.17).

Let us summarize the results for energy denominators: For core diagrams, and for the projecting core excitations of reduced valence diagrams, the "core" de-

nominators are simply

$$e_C = \sum_{\text{holes}} E_m - \sum_{\text{particles}} (E_\mu, E_b), \qquad (5.22)$$

exactly as in the Goldstone expansion. External valence particle lines must be ignored when evaluating e_C for reduced valence diagrams, although terms in which core particles scatter into valence states must be included. In the general case of quasi-degeneracy, the "valence" denominators are

$$e_V = E_{0V} + \Delta E_V + \sum (\text{all downgoing line energies}) - \sum (\text{all upgoing line energies}), \qquad (5.23)$$

where E_{0V} is given by (5.4).

"Valence Hole" Formulation

We have assumed that there are n valence particles beyond the closed shells, but for almost-filled shells it is more convenient to reformulate everything in terms of "holes." Thus one can begin by considering an N-particle core containing n' holes, the total number of particles being $N-n'$. (A "mixed" description is also possible, with n particles and n' holes.) There are three differences from the "valence particle" formulation: (a) The term E_{0V} of (5.4) and (5.23) now has the opposite sign, being the *negative* of the valence-state energies E_μ weighted by the *hole* probabilities $(1-P_\mu^{(0)})$. (b) The rule for determining the sign of a particular diagram is slightly different. This is discussed in Appendix B. (c) The precise statement of which states each line is to be summed over is different, but the guiding principle remains the same—the core diagrams must be the same as for the N-body problem, all others being considered valence diagrams.

VI. WAVE FUNCTIONS, EXPECTATION VALUES AND TRANSITION AMPLITUDES

Nondegenerate Case

The same techniques can be used to obtain a simple description of the wave functions, starting from $\Psi = \Omega\Psi_D$ and the expansion for Ω obtained by iterating (2.11). We first consider the nondegenerate case, $\Psi_D = \Phi_0$. A general diagram in the BW expansion for Ψ again consists of several overlapping linked parts. Some of these parts are "open", meaning that they have permanently created one or more particle–hole pairs. These pairs appear as external lines leaving and entering the top of the diagram. The remaining linked parts have the same "closed" form as those encountered in the energy expansion. In the present context these can be considered "vacuum fluctuations." The energy denominators are then converted from BW to RS form, by expanding out ΔE, and the diagram analysis then proceeds just as in the energy expansion. The only change is that the *principal part* now consists of *all* the open parts. After cancellation, one is again left with just the principal parts, all evaluated with RS energy denominators.

The most general diagram now consists of a number of open parts of each possible variety. These parts can be made independent of each other (put on the energy shell) by generalizing their relative "time" order and using the factorization theorem. Let n_r be the number of open parts $\mathbf{W}_r$ having topological form r. Then the factored diagram becomes

$$\left[\prod_r \frac{(\mathbf{W}_r)^{n_r}}{n_r!}\right] | \Phi_0\rangle. \qquad (6.1)$$

[The symbol $\mathbf{W}$ is suggested by the form of a typical open core diagram, as seen for example in (6.13).] The $(n_r!)^{-1}$ factors arise because, after summing over all single-particle indices, each possible relative time ordering (for each set of indices) is counted $n_r!$ times during the factorization process. Thus the sum of all diagrams is simply[29]

$$\Psi = \exp\{\sum_r \mathbf{W}_r\} | \Phi_0\rangle, \qquad (6.2)$$

where each variety of open part appears just once in the exponent. It should be emphasized that the open parts $\mathbf{W}_r$ are actually operators. An open part which creates p particle–hole pairs has the general form

$$\mathbf{W}_r(p) = \underbrace{\sum_{al}\sum_{bm}\cdots\sum_{cn}}_{p} W_r(al, bm, \cdots, cn) \times \eta_a^\dagger \eta_b^\dagger \cdots \eta_c^\dagger \eta_n \cdots \eta_m \eta_l. \qquad (6.3)$$

The algebraic steps leading to (6.1) and (6.2) are permissible because the $\mathbf{W}_r$ operators all commute with each other. The exponential expression (6.2) is convenient for formal purposes, and especially when N is large. For small N, it is useful to note that there is much cancellation in higher orders due to "exchange" terms. Thanks to these terms, one need not consider any diagrams of the form (6.1) which create more than N particle–hole pairs.

Assuming $\langle\Phi_0 | \Phi_0\rangle = 1$, it is easily verified that

$$\langle\Psi | \Psi\rangle = \langle\Phi_0 | [\exp \sum_s \mathbf{W}_s^\dagger][\exp \sum_r \mathbf{W}_r] | \Phi_0\rangle = \exp[-F_L'(E_0)], \qquad (6.4)$$

where

$$F_L(E_0) = \langle\Phi_0 | V \sum_{n=0}^{\infty} \left(\frac{Q}{E_0 - H_0} V\right)^n | \Phi_0\rangle_L = \Delta E \qquad (6.5)$$

is just Goldstone's linked-cluster energy expression. The prime on $F_L'(E_0)$ indicates differentiation with respect to E_0. Note that this derivative is negative, therefore $-F_L' > 0$. [To obtain (6.4), go back to the stage where Ψ and $\Psi^\dagger$ each consists of open parts,

$\mathbf{W}_r$ and $\mathbf{W}_s^\dagger$, which have not yet been factored. Connect up these open parts in all possible ways, and then apply the factorization theorem twice, to the $\mathbf{W}_r$'s and $\mathbf{W}_s^\dagger$'s separately. The symmetry factors $(n_r!)^{-1}$ will now refer to the numbers n_r of *closed* parts with the same topological form.] This result was obtained first by Hugenholtz[29] and then by Bloch.[30] It is clear that $\Delta E \propto N$ for a large saturating system, thus (6.4) demonstrates that the probability of finding the system in its "model state" Φ_0 is $\sim e^{-\alpha N}$. This is to be expected on physical grounds,[47,29] as discussed in Sec. IX.

The complete wave function of a many-body system is extremely complicated, but expectation values fortunately take on a much simpler form. Consider a general n-body operator

$$\mathcal{O}(n)=(n!)^{-1}\underbrace{\sum_{ij}\sum_{i'j'}\cdots\sum_{i''j''}}_{n}\mathcal{O}(ij,i'j',\cdots i''j'')\times\eta_i^\dagger\eta_{i'}^\dagger\cdots\eta_{i''}^\dagger\eta_{j''}\cdots\eta_{j'}\eta_j, \quad (6.6)$$

where the indices i, j range over *all* single-particle states, including both "particle" and "hole" states. (The $n!$ divisor compensates for the unrestricted summations, so that each distinct term is included only once.) The procedure leading to (6.2) will also give $\mathcal{O}\Psi$ if the *last* (topmost) interaction is always taken to be $\mathcal{O}$. Each diagram will have just one open (or possibly closed) part $(\mathcal{O}\mathbf{W})_r$ containing $\mathcal{O}$, therefore

$$\mathcal{O}\Psi=\sum_r(\mathcal{O}\mathbf{W})_r[\exp\sum_s\mathbf{W}_s]\,|\,\Phi_0\rangle. \quad (6.7)$$

[The $(\mathcal{O}\mathbf{W})_r$ part might consist of several $\mathbf{W}$ parts joined together by $\mathcal{O}$.] Note that $\mathcal{O}$ is able to create or absorb up to n particle–hole pairs, but that $(\mathcal{O}\mathbf{W})_r$ can, by definition, only *create* pairs. Thus $(\mathcal{O}\mathbf{W})_r$ commutes with the $\mathbf{W}_s$'s. The exponential occurs in (6.7) because symmetry factors $(n_s!)^{-1}$ still arise for those parts $\mathbf{W}_s$ which are not attached to $\mathcal{O}$. By similar arguments one easily finds[62]

$$\langle\Psi\,|\,\mathcal{O}\,|\,\Psi\rangle=\langle\Phi_0\,|\,[\exp\sum_t\mathbf{W}_t^\dagger]\sum_r(\mathbf{W}^\dagger\mathcal{O}\mathbf{W})_r\times[\exp\sum_s\mathbf{W}_s]\,|\,\Phi_0\rangle$$
$$=\langle\Psi\,|\,\Psi\rangle\langle\Phi_0\,|\,\sum_r(\mathbf{W}^\dagger\mathcal{O}\mathbf{W})_r\,|\,\Phi_0\rangle, \quad (6.8)$$

and therefore

$$\langle\mathcal{O}\rangle\equiv\langle\Psi\,|\,\mathcal{O}\,|\,\Psi\rangle/\langle\Psi\,|\,\Psi\rangle=\langle\Phi_0\,|\,\sum_r(\mathbf{W}^\dagger\mathcal{O}\mathbf{W})_r\,|\,\Phi_0\rangle. \quad (6.9)$$

This factorization is possible because of two circumstances: (1) each term $(\mathbf{W}^\dagger\mathcal{O}\mathbf{W})_r$ is "closed," by definition, meaning that it refills exactly the same set of hole states (m states) that it has previously emptied. Factorization would follow from this alone, were it not for the exclusion principle. (2) For each term in (6.8) where an $\mathcal{O}$ diagram and a normalization diagram both empty the same m state, or both fill the same b state (particle state), there is a corresponding exchange term among the set of $\mathcal{O}$ diagrams whose contribution is exactly equal and opposite. *Thus one must consistently neglect exclusion. The expectation value* $\langle\mathcal{O}\rangle$ *is therefore given by the sum of all linked diagrams in which* $\mathcal{O}$ *appears just once.* This simple result is due to Thouless,[42,43] and was also obtained by Glassgold, Heckrotte, and Watson.[63] Da Providencia[64] has found a very similar expression for a general antisymmetric Ψ, a variational wave function for example, without relying on perturbation-theoretic arguments.

One can also argue[63,65] that this simple result is a direct consequence of the energy expansion. Let the perturbation V be replaced by $V+\lambda\mathcal{O}$. By comparing the Schrödinger equations for $\lambda=0$ and $\lambda\neq0$, one finds immediately that

$$\lambda\langle\Psi_{\lambda=0}\,|\,\mathcal{O}\,|\,\Psi_\lambda\rangle=[E(\lambda)-E(\lambda=0)]\langle\Psi_{\lambda=0}\,|\,\Psi_\lambda\rangle, \quad (6.10)$$

and therefore

$$\langle\mathcal{O}\rangle=\lim_{\lambda\to0}\frac{E(\lambda)-E(\lambda=0)}{\lambda}. \quad (6.11)$$

(This is essentially the Feynman theorem.[66]) The argument is concluded by observing that since λ can be arbitrarily small, it is only necessary to consider the "energy" diagrams in which $\mathcal{O}$ appears just once. This also shows that the rules for the $\langle\mathcal{O}\rangle$ diagrams are essentially the same as those for ΔE (see Appendix B).

We have already mentioned that one can neglect all terms in (6.1) which contain more particle–hole pairs than the total number of particles in the system. More generally, one can consistently neglect all terms in the *unlinked* expansion (6.1) in which the *external* lines violate exclusion. But of course this is *not* allowed in the linked expansions for ΔE, $\langle\Psi\,|\,\Psi\rangle$, and $\langle\mathcal{O}\rangle$, where the exclusion violating terms must be retained. Their physical significance is discussed in Sec. IX.

Degenerate Case

We shall begin by assuming strict degeneracy, although, by the argument of (5.17), the results must also apply to the quasi-degenerate case. Working in the $\mathbf{A}_\beta^{(\alpha)}$ representation, one finds that the BW diagrams in $\Psi=\Omega\Psi_D$ may each contain an overlapping valence *group* which is open at the top. Each diagram may also contain an arbitrary number of open core parts, $\mathbf{W}_r$, which are identical to those considered above.

[62] There is a slight ambiguity in our notation. The set of W's and $\mathbf{W}^\dagger$'s in $(\mathbf{W}^\dagger\mathcal{O}\mathbf{W})$ should be thought of as including the unit operator, although this does not appear in the exponent of (6.2).

[63] A. E. Glassgold, W. Heckrotte, and K. M. Watson, Phys. Rev. **115**, 1374 (1959).

[64] J. DaProvidencia, Nucl. Phys. **46**, 401 (1963).

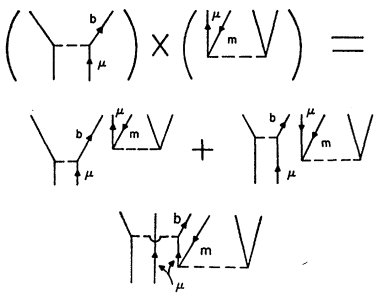
[65] E. Daniel and S. H. Vosko, Phys. Rev. **120**, 2041 (1960).

[66] R. P. Feynman, Phys. Rev. **56**, 340 (1939).

Just as in the energy expansion, the removal of ΔE_C and ΔE_V (where appropriate) from the energy denominators eliminates all diagrams containing "vacuum fluctuations", i.e., closed core parts or closed valence groups. The factorization theorem then gives

$$\Psi=\sum_r \mathbf{Y}_r[\exp\sum_s \mathbf{W}_s]\,|\,\Psi_D\rangle. \tag{6.12}$$

The $\mathbf{Y}_r$'s are the open valence groups, examples of which appear in (6.13) and (6.14). Their sum must include the [$(N+n)$-body] unit operator, $\mathbf{Y}_0\equiv I$. The *bottom* parts of many of these valence groups can be simplified, or "reduced," through the cancellation shown in (5.18). The open core parts $\mathbf{W}_s$ are defined as in (6.3). They may excite core particles into valence states μ as well as into the intermediate states b. Exclusion-violating terms occur whenever a core particle (from $\mathbf{W}$) and a valence particle (from $\mathbf{Y}$) are in the same single-particle state (μ or b), or when $\mathbf{W}$ and $\mathbf{Y}$ terms both empty the same m state. These terms should be included, since they are compensated by "c-v exchange" terms which appear among the other $\mathbf{Y}_r$'s. As an example, the last term in (6.13) is cancelled by (6.14).



(6.13)

(6.14)

We have met similar terms before, in (5.9). Thanks to these c-v exchange terms, one can safely assume that the $\mathbf{W}_s$'s and $\mathbf{Y}_r$'s all commute. [This is essentially the same argument used to justify the factorization in (6.8).]

We express the separation of ΔE into core and valence terms as follows:

$$\begin{aligned}\Delta E&=\langle\Psi_D\,|\,\mathcal{U}\,|\,\Psi_D\rangle_C+\langle\Psi_D\,|\,\mathcal{U}\,|\,\Psi_D\rangle_V\\&=F_{CL}(E_{0C})+F_V(E_{0V}+\Delta E_V)\\&=\Delta E_C+\Delta E_V.\end{aligned} \tag{6.15}$$

This $F_{CL}(E_{0C})$ is identical, of course, to (6.5). The normalization can then be put in the form

$$\begin{aligned}\langle\Psi\,|\,\Psi\rangle&=\langle\Psi\,|\,\Psi\rangle_C\langle\Psi\,|\,\Psi\rangle_V\\&=\{\exp[-F_{CL}'(E_{0C})]\}[1-F_V'(E_{0V}+\Delta E_V)],\end{aligned} \tag{6.16}$$

(assuming $\langle\Psi_D\,|\,\Psi_D\rangle=1$), following the logic of (6.8), (6.13), and (6.14). If "reduced" valence groups are used, the argument $(E_{0V}+\Delta E_V)$ in the F_V and F_V' terms must be replaced by E_{0V} at the levels of projecting core excitations, i.e., the "valence" denominators (5.23) are replaced by "core" denominators (5.22).

It is useful to indicate the state dependence of various quantities more explicitly:

$$\Psi_\alpha=\Omega_\alpha\Psi_{D\alpha}=\sum_{j\in D} a_{\alpha j}\Omega_\alpha\Phi_j, \tag{6.17}$$

$$\Omega_\alpha=[\exp\sum_s \mathbf{W}_s]\sum_r \mathbf{Y}_r(E_{0V\alpha}+\Delta E_{V\alpha}), \tag{6.18}$$

$$\langle\Psi_\alpha\,|\,\Psi_\alpha\rangle=N_\alpha=N_C N_{V\alpha}, \tag{6.19}$$

$$N_C=\exp[-F_{CL}'(E_{0C})], \tag{6.20}$$

$$\begin{aligned}N_{V\alpha}&=\langle\Psi_{D\alpha}\,|\,[1-\mathcal{U}_V'(E_{0V\alpha}+\Delta E_{V\alpha})]\,|\,\Psi_{D\alpha}\rangle\\&=1-F_V'(E_{0V\alpha}+\Delta E_{V\alpha}).\end{aligned} \tag{6.21}$$

Thus one can write

$$\begin{aligned}\langle\Psi_\beta\,|\,\mathcal{O}\,|\,\Psi_\alpha\rangle&=\langle\Psi\overset{\frown}{|}\Psi\rangle_C\langle\Psi_\beta\,|\,\mathcal{O}\,|\,\Psi_\alpha\rangle_V\\&\quad+\langle\Psi\,|\,\overset{\frown}{\mathcal{O}}\,|\,\Psi\rangle_C\langle\Psi_\beta\,|\,\Psi_\alpha\rangle_V\\&=N_C[\langle\Psi_\beta\,|\,\mathcal{O}\,|\,\Psi_\alpha\rangle_V+\delta_{\beta\alpha}N_{V\alpha}\langle\mathcal{O}\rangle_C],\end{aligned} \tag{6.22}$$

by again separating the diagrams into two sets, those in which $\mathcal{O}$ interacts with a valence group and those in which it does not. Each set is then factored into core and valence terms, as in (6.16). (No subscripts are needed for the Ψ's appearing in the "core" factors, since these consist entirely of core diagrams.) From this one obtains both the expectation values $\langle\alpha\,|\,\mathcal{O}\,|\,\alpha\rangle$, and off-diagonal "transition" matrix elements

$$\begin{aligned}\langle\beta\,|\,\mathcal{O}\,|\,\alpha\rangle&=\langle\Psi_\beta\,|\,\mathcal{O}\,|\,\Psi_\alpha\rangle/(N_\beta N_\alpha)^{1/2}\\&=\langle\Psi_\beta\,|\,\mathcal{O}\,|\,\Psi_\alpha\rangle_V/(N_{V\beta}N_{V\alpha})^{1/2}+\delta_{\beta\alpha}\langle\mathcal{O}\rangle_C.\end{aligned} \tag{6.23}$$

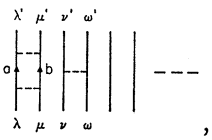
The most general term in $\langle\Psi_\beta\,|\,\mathcal{O}\,|\,\Psi_\alpha\rangle_V$ consists of a single $\mathbf{Y}$ and several $\mathbf{W}$'s below the $\mathcal{O}$ interaction, and above this a single $\mathbf{Y}^\dagger$ with several $\mathbf{W}^\dagger$'s, all connected together to form a single linked diagram. The $\mathbf{W}$'s and $\mathbf{W}^\dagger$'s can all be factorized and put on the energy shell. This involves the trick, mentioned below (5.19), of associating an additional excitation energy of $\Delta E_{V\alpha}$ (or $\Delta E_{V\beta}$) with the δE_j corresponding to the lowest (highest) valence interaction in $\mathbf{Y}(\mathbf{Y}^\dagger)$. The denominators of the $\mathbf{Y}$'s and $\mathbf{Y}^\dagger$'s contain $(E_{0V}+\Delta E_V)_\alpha$ $(E_{0V}+\Delta E_V)_\beta$, respectively, except where these have been reduced. The last term, $\langle\mathcal{O}\rangle_C$, is just the expectation value of $\mathcal{O}$ for the closed-shell nucleus obtained by physically removing the valence particles. [It might appear that (6.22) and (6.23) are both wrong by a factor of 2 when $\mathcal{O}$ is the unit operator. This little paradox is resolved by noting that the "unit operator" must in this case be an $(N+n)$-body operator, in the sense of (6.6), so that $\langle\mathcal{O}\rangle_C$ is now zero.] The unsymmetrical treatment of core and valence particles causes the valence normalization factors $N_{V\alpha}$, $N_{V\beta}$ to appear explicitly in (6.23). These factors are nontrivial even

in the apparently simple case where $n=1$, because they include effects of correlations between core and valence particles. In the next section we present a "completely linked" expansion for $\langle\beta \mid \mathcal{O} \mid \alpha\rangle$, in which these factors do not occur explicitly.

A striking feature of these "degenerate" results is that they all consist of terms describing the isolated N-body system, plus other terms describing the *changes* due to the *physical addition* of the n valence particles. These latter terms are closely related to n-body Green's functions. More specifically, they resemble the Hugenholtz[29] propagators $\bar{D}_\alpha$ rather than the causal Green's functions. This is because, just as in the Hugenholtz study, we have concentrated attention on the exact eigenstates instead of on the time dependence of nonstationary states. Nevertheless, we believe that most of these results, such as (6.15) for ΔE_V, will remain valid for quasi-stationary states with a comparatively long lifetime. In this case one should simply look for solutions where the energy eigenvalues have small imaginary parts. A better procedure is available for states with a stronger and more complicated time dependence. This is described in Sec. VIII.

VII. LINKED VALENCE EXPANSIONS

The valence terms of Secs. V and VI still retain many features of the original starting point, the BW expansions of Sec. II. The valence denominators (5.23) still contain ΔE_V, and the sets of diagrams include many unlinked terms. These features may not be too objectionable for small n. When there are many valence particles, however, they lead to the same kind of difficulties one finds in applying the BW theory to a nondegenerate many-body system. As an extreme example, one can regard the superfluid state of nuclear matter as the limiting form of the pairing phenomenon in very large nuclei. Bell[67] has already pointed out that the Bloch–Horowitz expansion is not suitable for this limiting case. In very large nuclei the ratio n/N should approach a small but finite limit (if we assume that the actual nuclear-matter ground state is weakly superfluid), thus $\Delta E_V \propto n \propto N$ can eventually become arbitrarily large. It would be senseless to use energy denominators containing such large energy shifts. Furthermore, the BH expansion contains unlinked terms such as (7.1),



, (7.1)

which that formalism would have to describe as an effective four-body interaction.

The arguments of Secs. IV and V lead us to expect a high degree of cancellation between these unlinked diagrams and those obtained by expanding ΔE_V out of the energy denominators. This possibility was first recognized by Morita,[49] who also sought to demonstrate this cancellation. Unfortunately, his final result is vague and misleading. We shall complete this program using the methods of the preceding sections, with modifications suggested by Morita's work. The task is considerably more difficult than in the nondegenerate case. It may be helpful to see, first of all, just where the previous methods fail.

Let us review the steps we would follow to convert the nondegenerate BW expansion, in terms of diagrams with N external lines, into the Goldstone expansion. (i) We would replace the external-line graphs by "vacuum" diagrams similar to Goldstone's. (ii) The exclusion principle must then be disregarded when summing each particle (hole) line over all particle (hole) states. This does no harm, as long as one is consistent, because the resulting exclusion-violating terms always occur in pairs (the members of which will be found in separate diagrams) which exactly cancel each other. This has the important advantage of making each linked part identical, with regard to its single-particle summations, to another complete diagram in the ΔE expansion. (iii) Finally, the energy shifts are expanded out of the BW denominators, and the argument of Sec. IV is used to eliminate unlinked terms.

The degenerate case is rendered much more difficult by the fact that the state $\mathbf{A}_\alpha$, used as a "vacuum state" to separate the core and valence terms, does not provide a useful "vacuum" description for the individual $(\mathcal{U}_V)_{ij}$ elements. The above program fails already in step (i). Another symptom of this difficulty is that the concept of "linked valence part," as used here with respect to the Φ_i basis for D, is not quite the same as in Secs. V and VI, where the linked parts were defined by $\mathbf{A}_\alpha$. The situation is simple only when the number of valence particles, n, is just equal to the number of valence states. In this case $d=1$, so the system is actually nondegenerate. The above steps (i), (ii), and (iii) can then be used, with slight modifications, to convert the n-external-line $\mathcal{U}_V$ diagrams into a set of linked diagrams which are just the difference between the Goldstone expansions for the N-body and the $(N+n)$-body systems.

Another difficulty arises in step (iii). In the nondegenerate case one finds, after ignoring exclusion, that each linked part resembles a complete diagram in the ΔE expansion. But for $d>1$ we find that $\Delta E_V = \mathbf{A}^\dagger \mathcal{U}_V \mathbf{A}$ involves all d^2 different $(\mathcal{U}_V)_{ij}$ matrix elements, each of which has a weighting factor $a_i^* a_j \neq 1$. Starting with a particular $(\mathcal{U}_V)_{ij}$ element and expanding out ΔE_V, we find all the other elements appearing. Worse still, the problems of calculating $\mathcal{U}_V$ and $\mathbf{A}$ now seem to be hopelessly intermixed.

[67] J. S. Bell, Ref. 20.

Matrix Multiplication

The clue to the solution can be found in Morita's work.[49] We shall start from quite a different viewpoint, however, and establish contact with his method at a later stage. Starting with the *reduced* Bloch–Horowitz expansion for $\mathcal{U}_V$, let us expand ΔE_V out of the denominators as in (3.6). [Again we assume exact degeneracy, with all valence-state energies equal to $\bar{E}_\mu$, and wait until the very end to remove this restriction by the argument of (5.17).] Let us collect together all terms of $\mathcal{U}_V$ which contain exactly r insertions of $(-\Delta E_V)$. We denote their sum by

$$\mathcal{U}_V{}^{(r)}[-\Delta E_V]^r, \tag{7.2}$$

so that

$$\mathcal{U}_V(E_{V\alpha})=\sum_{r=0}^{\infty}\mathcal{U}_V{}^{(r)}[-\Delta E_{V\alpha}]^r$$

$$=\sum_{r=0}^{\infty}\mathcal{U}_V{}^{(r)}[-\mathbf{A}_\alpha{}^{(\alpha)\dagger}\mathcal{U}_V(E_{V\alpha})\mathbf{A}_\alpha{}^{(\alpha)}]^r. \tag{7.3}$$

The denominators in $\mathcal{U}_V{}^{(r)}$ are basically of *RS* form, E_0-H_0, which in this case means

$$(e_V)_{\mathrm{RS}}=n\bar{E}_\mu+\sum\text{ (downgoing line energies)}$$
$$-\sum\text{ (upgoing line energies)}. \tag{7.4}$$

The $\mathcal{U}_V(E_{V\alpha})$'s in (7.3) are still given by the BH prescription, with ΔE_V remaining in their denominators.

Now, since $\mathcal{U}_V(E_{V\alpha})$ is diagonal in the $\mathbf{A}_\alpha{}^{(\alpha)}$ representation [see (5.8)], we see immediately that

$$\mathcal{U}_V(E_{V\alpha})\mathbf{A}_\alpha{}^{(\alpha)}=\sum_{r=0}^{\infty}\mathcal{U}_V{}^{(r)}[-\mathcal{U}_V(E_{V\alpha})]^r\mathbf{A}_\alpha{}^{(\alpha)}. \tag{7.5}$$

This suggests the introduction of a new matrix,

$$\mathcal{W}_1(\alpha)\equiv\sum_{r=0}^{\infty}\mathcal{U}_V{}^{(r)}[-\mathcal{U}_V(E_{V\alpha})]^r. \tag{7.6}$$

We see from (7.5) that $\mathbf{A}_\alpha{}^{(\alpha)}$ is also an eigenvector of $\mathcal{W}_1(\alpha)$, with the same eigenvalue $\Delta E_{V\alpha}$. This will allow us to use (7.6) in place of $\mathcal{U}_V$ in the secular equation (5.13). After this replacement, the new set of eigenvectors and eigenvalues will include the desired A_α and $E_{V\alpha}$. Note, however, that

$$\mathcal{W}_1(\alpha)\mathbf{A}_\beta{}^{(\alpha)}=\sum_{r=0}^{\infty}\mathcal{U}_V{}^{(r)}\mathbf{A}_\beta{}^{(\alpha)}[-\mathbf{A}_\beta{}^{(\alpha)\dagger}\mathcal{U}_V(E_{V\alpha})\mathbf{A}_\beta{}^{(\alpha)}]^r$$

$$=\sum_{r=0}^{\infty}\mathcal{U}_V{}^{(r)}[-\Delta E_V{}^{(\alpha)}{}_\beta]^r\mathbf{A}_\beta{}^{(\alpha)}$$

$$=\mathcal{U}_V(n\bar{E}_\mu+\Delta E_V{}^{(\alpha)}{}_\beta)\mathbf{A}_\beta{}^{(\alpha)}, \tag{7.7}$$

which shows that the matrices $\mathcal{U}_V(E_{V\alpha})$ and $\mathcal{W}_1(\alpha)$ are generally not identical. [See (5.8) for notation.]

Repetition of these arguments leads to a matrix with "second-generation" insertions,

$$\mathcal{W}_2(\alpha)\equiv\sum_{r=0}^{\infty}\mathcal{U}_V{}^{(r)}[-\mathcal{W}_1(\alpha)]^r$$

$$=\sum_r\mathcal{U}_V{}^{(r)}\{-\sum_{s_1}\mathcal{U}_V{}^{(s_1)}[-\mathcal{U}_V(E_{V\alpha})]^{s_1}\}\times\cdots$$
$$\times\{-\sum_{s_r}\mathcal{U}_V{}^{(s_r)}[-\mathcal{U}_V(E_{V\alpha})]^{s_r}\}. \tag{7.8}$$

It should be clear that the desired $\mathbf{A}_\alpha$ and $E_{V\alpha}$ can still be obtained when this is used in the secular equation. Suppose we repeat this process η times, using the BH expansion for the "ηth-generation" $\mathcal{U}_V(E_{V\alpha})$'s to complete the perturbation expansion for $\mathcal{W}_\eta(\alpha)$. One can easily check [consider sequences of second-order insertions such as (3.10)] that $\Delta E_{V\alpha}$ will not appear in any term of order less than $2(\eta+1)$. In other words, the first $2\eta+1$ orders of $\mathcal{W}_\eta(\alpha)$ form a degenerate version of the RS perturbation series. The factorization theorem then leads to a degenerate analogue of the Goldstone expansion. We see that the problem of the weighting factors $a_i{}^*a_j$ in $\Delta E_V=\sum_{ij}a_i{}^*a_j(\mathcal{U}_V)_{ij}$ has been solved by combining the various elements of $\mathcal{U}_V$ in a simple way. Before we can demonstrate the cancellation of unlinked terms, however, we must find a suitable diagrammatic description for this "degenerate Goldstone expansion" corresponding to $\mathcal{W}_\infty$.

First, let us remark that the desired eigenvalue $E_{V\alpha}$ or $\Delta E_{V\alpha}$ still appears within (7.8) and all its "higher-generation" analogues. In a weakly perturbed system where everything converges, use of the complete $\mathcal{W}_\eta$ for any finite η will preserve the peculiar lack of complete orthogonality among the true $\mathbf{A}_\alpha$ eigenvectors. The limiting form $\mathcal{W}_\infty$ will also give the $\mathbf{A}_\alpha$'s correctly. We presume that this remains true even for strongly interacting systems such as nuclei. For a reasonable choice of the subspace D, the usual analytic continuation arguments should be as valid here as for the nondegenerate problem of closed shells. This is discussed further in Sec. IX. Thus it should be possible to obtain reasonable approximations for $\mathcal{W}_\infty$, including its nonorthogonal aspects, by considering valence diagrams which are the natural analogues of those used for the closed shells. The *true* nonorthogonality of the $\mathbf{A}_\alpha$'s is probably very weak, however, in many applications, and it might require a very careful treatment to detect this. Formal aspects of this nonorthogonality are discussed in Appendix D.

Folded Diagrams

The perturbation expansion of $\mathcal{W}_\infty$ can best be represented by diagrams of a new type suggested by Goldstone's adiabatic approach. Morita was the first to observe this, and this is the appropriate place to establish contact with his work. In the present deriva-

tion we do not actually rely on adiabatic arguments at any stage. Nevertheless, it is worthwhile to understand the connections with this other approach.

It will suffice to consider how the adiabatic method applies to the simple "one particle in an external field" model of Sec. III. One generates an adiabatic wave function

$$\Psi_\epsilon' = U_\epsilon(0, -\infty)\Phi_0, \tag{7.9}$$

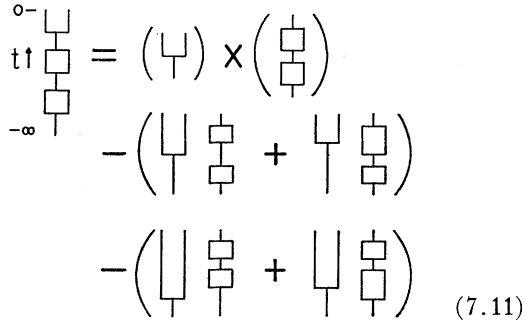
by switching on the interaction at a very slow rate, ϵ, over the time interval $-\infty < t < 0$. The result can be expressed as

$$\Psi_\epsilon' = \Psi_\epsilon \langle \Phi_0 \mid U_\epsilon(0, -\infty) \mid \Phi_0 \rangle, \tag{7.10}$$

where Ψ_ϵ has a well-defined limit as $\epsilon \to 0$. This limit is just the desired wave function $\Psi = \Omega\Phi_0$, normalized so that $\langle \Phi_0 \mid \Psi \rangle = 1$. The unwanted factor $\langle \Phi_0 \mid U_\epsilon \mid \Phi_0 \rangle$ consists of a normalization factor $(\langle \Psi_\epsilon \mid \Psi_\epsilon \rangle)^{-1/2}$ (since U_ϵ is a unitary operator) whose form is similar to (6.4), as well as an unobservable phase factor whose limit is undefined as $\epsilon \to 0$. [This result is obtained by expanding the products of the adiabatic energy denominators $(e + in'\epsilon)^{-1}$ in powers of ϵ, keeping both the zero and first-order terms.] The phase factor is $\exp\{\sum_n (\Delta E^{(n)}/in\epsilon)\}$, where $\Delta E^{(n)}$ is the sum of all nth order terms in ΔE. It corresponds physically to

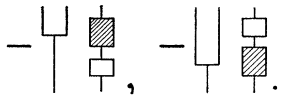
$$\exp\{-i\int_{-\infty}^{0} \Delta E(t)\, dt\}.$$

Now the object is to perform this factorization, (7.10), diagram by diagram. The first step is to relax certain of the time-order restrictions, and then to explicitly subtract the new terms which arise. This is illustrated for a typical Ψ_ϵ' diagram in (7.11).



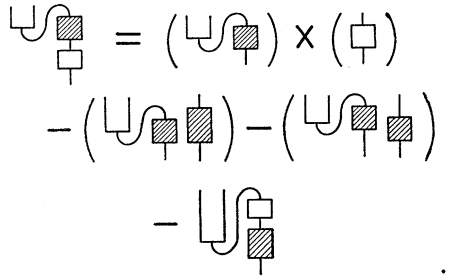
(7.11)

Here the lines refer to the vacuum state Φ_0, and the boxes to "interaction blocks" within which Φ_0 does *not* appear as an intermediate state. We shall simplify the notation a little, expressing the last two brackets of (7.11) as



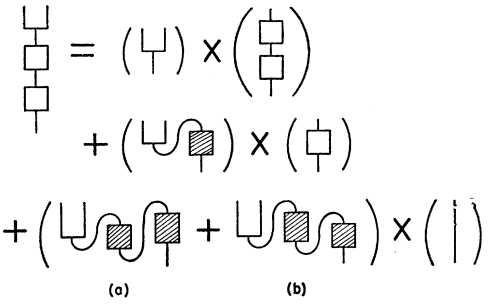
(7.12)

The shaded rectangle indicates all possible time-orderings of that block with respect to the "principal part" (topmost block), with the single restriction that the topmost interaction of the shaded rectangle be kept in the same position as in (7.11). We now introduce "folded vacuum lines" to indicate factors of (-1). Using this convention, the first term in (7.12) can also be factored:



(7.13)

The last term in (7.13) cancels the second term in (7.12), so the final result is



(7.14)

This argument indicates that the Ψ_ϵ' diagrams can all be reduced to a sum of terms in which Ψ_ϵ diagrams are multiplied by $\langle \Phi_0 \mid U_\epsilon \mid \Phi_0 \rangle$ diagrams.

The Ψ_ϵ diagrams all consist of a principal part and a number of insertions, all linked together by "folded vacuum lines" such that *the top of each insertion occurs above the bottom of the preceding insertion.* These diagrams remain well-defined in the limit $\epsilon \to 0$, and they can be used in our purely algebraic context without reference to any adiabatic process. A similar "folded string of beads" form can be used for the diagrams of $\Delta E = \langle \Phi_0 \mid V \mid \Psi \rangle = \langle \Phi_0 \mid \mathcal{V} \mid \Phi_0 \rangle$. Thus, diagram (a) of (7.14) corresponds to two "first generation" insertions, in other words to the $r=2$ term in (7.6), whereas diagram (b) introduces a "second generation", as in (3.10) and (7.8). These folded diagrams for ΔE are completely equivalent to the closed-loop Goldstone diagrams of Sec. III. The one-to-one correspondence is established by noting that the folded diagrams are obtained by cutting the downgoing "hole" line attached to the *topmost* interaction of the closed-loop diagrams. (This correspondence is worth studying carefully, to see in detail how the various "generations" of insertions are represented by the "folded" topology. Another example of this topology is shown in Fig. 6 of Ref. 9.)

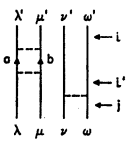
This folded form is exactly what we need for a degenerate one-body system. Each "vacuum line"

acquires a label referring to one of the degenerate Φ_i's, and the matrix multiplication in (7.6) is performed by simply summing the internal (folded) vacuum lines over all indices $i \in D$. The external lines are *not* summed. They specify which element i, j of $\mathfrak{W}_\infty$ the diagram belongs to.

Let us return for a moment to the adiabatic method. For a nondegenerate N-body system one begins, of course, with the vacuum convention for representing Φ_0, instead of the N-external line convention implied by (7.11). The addition and subtraction of terms which (7.11) illustrates is then accomplished quite automatically when one drops the exclusion restrictions among hole lines. The folded diagrams correspond to the exclusion-violating Goldstone diagrams with two or more holes in the same normally occupied state m. (When $N=1$, of course, all diagrams with more than one hole line fall into this category. This should be clear from Sec. III.) We mention this because the folded diagrams for the degenerate case cannot be obtained in quite such a blindly mechanical fashion, for lack of a suitable vacuum convention, and it becomes important to understand their folded structure in detail. With Morita's adiabatic approach, for example, it is necessary to follow through the arguments (7.11) to (7.14) explicitly.

Linked Expansion for $\mathfrak{V}_V$

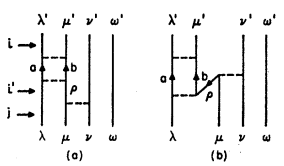
We come at last to the valence diagrams for a degenerate many-body system. Each "one-body" folded diagram is replaced by a set of n-external-line diagrams, all of which have the same folded structure. Consider the case of $n=4$. There is an $r=1$ term of (7.6) which can be drawn in *unfolded* form as



(7.15)

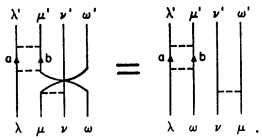
Thanks to the factor of $(-1)^r$, this will cancel the unlinked term similar to (7.1). All other unlinked valence diagrams are eliminated in the same way, as shown below. But the exclusion principle might appear to create difficulties here. The matrix multiplication requires us to sum (7.15) over all degenerate states i'. This implies that the indices ν', ω' should not coincide with either λ or μ, whereas there is no such restriction in (7.1).

Now consider the $r=1$ term shown in (7.16) in both unfolded and folded form.



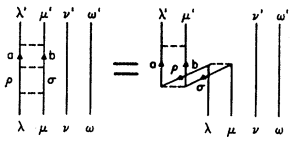
(7.16)

The i' summation in (a) implies, together with the exclusion principle, that ρ should not coincide with ν', ω', or λ. But we can drop this restriction if we also include the corresponding exchange terms. For the case where $\rho=\omega=\omega'$, the required exchange term is



(7.17)

Except for a permutation of the $(\lambda\mu\nu\omega)$ labels, this is just the $\mu=\omega'$ term which must be added to (7.15) to cancel the corresponding term in (7.1). [One must eventually consider all permutations of the indices $(\lambda\mu\nu\omega)$ and $(\lambda'\mu'\nu'\omega')$.] The $\rho=\lambda$ and $\rho=\nu'$ terms in (7.16) happen, in this case, to be cancelled by other terms with the same topological form as (7.16). Exclusion also requires that $\lambda \neq \nu'$ in (7.16), but this can be cancelled by the $\rho=\nu=\nu'$ term in (7.18).



(7.18)

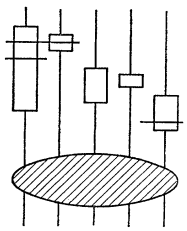
The $\rho=\nu=\nu'$, $\sigma=\omega=\omega'$ term of (7.18) is also needed, to cancel the $\lambda=\nu'$, $\mu=\omega'$ term in (7.1).

These examples demonstrate that one should, quite generally, ignore exclusion principle restrictions among the folded valence lines. These lines should simply be summed, independently, over all valence states μ. This is necessary to complete the elimination of unlinked diagrams. It has the additional advantage of making the noninteracting valence lines, such as the $\omega=\omega'$ lines in (7.16) and (7.18), entirely superfluous. Thus, one need draw only those parts of diagrams which are *completely linked*, and which have $\leq n$ external lines. The general validity of these statements follows from the fact that the Wick algebra automatically preserves antisymmetry at *each* intermediate-state level where it is used consistently, regardless of whether the level is degenerate or not. It is convenient to take exclusion into account in labelling the external lines, but to ignore this in *all* intermediate states of the *unfolded* diagrams.

We shall now demonstrate that *all* of the unlinked terms in $\mathfrak{W}_\infty$ cancel each other. The proof is very similar to the one given in Sec. IV for the Goldstone expansion. Consider the *unfolded* forms of the diagrams for $\mathfrak{W}_\infty$. If a particular diagram contains more than one $\mathfrak{V}_V$ block (a diagram with one or more folds), the *highest* of these blocks will contain one or more levels with repeated energy denominators. The highest block is therefore a term in $\mathfrak{V}_V^{(r)}$ [see (7.2)] with $r \geq 1$. Draw r horizontal bars through this block to indicate the locations of the repeated energy denominators. The entire diagram now corresponds to a diagram like (4.6)

containing r insertions of $(-\Delta E_V)$, except that each of these insertions is now represented by a specific term in its expansion, as in (3.7).

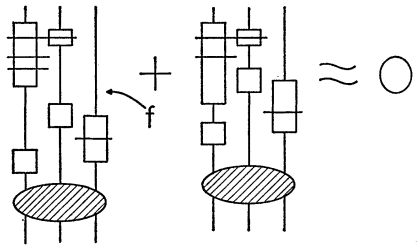
The next step is to identify the "principal part" and the "overlapping groups" for this diagram. The principal part is now the linked part of the topmost $\mathcal{U}_V$ block which contains the topmost interaction of the entire diagram. If the topmost $\mathcal{U}_V$ block contains any other linked parts, these can be organized into overlapping groups, exactly as Sec. IV. Finally, these overlapping groups and the r horizontal bars can be organized into "time blocks". A $\mathcal{W}_\infty$ diagram with exactly the same structure as (4.6) is shown schematically in (7.19).



(7.19)

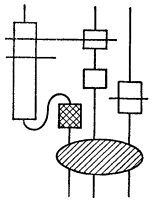
Each vertical line here may represent more than one valence particle. The shaded blob represents all of the other $\mathcal{U}_V$ blocks, in other words the insertions. (There may be more than r of these blocks, since each of the r insertions may itself contain insertions.)

The next step should be obvious. An example which corresponds to (4.7) is shown in (7.20).



(7.20)

The lowest overlapping group on the right-hand side is cancelled by a similar diagram in which this group now appears as the highest insertion. The "f" on the left-hand side is to indicate the presence of an extra fold. We have written ≈ 0 because, after doing the fold "f" explicitly, and factorizing the insertion, the left-hand diagram is found to include some extra terms. These have the form shown in (7.21).



(7.21)

To eliminate this term we must repeat all the preceding steps, but with the cross-hatched part included now within the definition of the principal part. This complication arises again and again, but any unlinked diagram of finite order can be cancelled completely by repeating this procedure a finite number of times. This difficulty is a reflection of the fact that we began here with a definition of the principal part which differs from the definition given in Sec. IV. In a *closed* diagram, the principal part already includes an arbitrary number (≥ 0) of these folded-in insertions. [The closed principal parts with folded insertions are all similar to (4.8a), with one or more pairs of crossed hole lines carrying the same index. Thus there may be two-body, three-body, $\cdots$, n-body insertions, i.e., insertions attached by any number of crossed pairs of hole lines.]

The proof is completed by noting that the projecting core excitations all factorize automatically, since we began here with the *reduced* form of the Bloch–Horowitz expansion. The projecting core excitations may therefore be ignored for the purposes of the present argument. (They should be regarded simply as numerical factors, with no vertical extension.) The "time" limits of each of the $\mathcal{U}_V$ pieces, i.e., the levels at which the valence lines are folded, are determined by the valence interactions alone. It should be clear that this general folded structure offers much opportunity to simplify the remaining linked diagrams by further factorizations.

Diagram Rules

The derivation is now complete except for a statement of the diagram rules.[68,69] To minimize confusion, we shall make a fresh start instead of merely listing the alterations of the Bloch–Horowitz rules given in Appendix B. There are many details to keep track of, and it will be useful to consider both the "folded" and the "unfolded" form of each diagram.

1. Topology

The most general diagram can be constructed as follows: Draw an arbitrary number $(f+1)$ of Bloch–Horowitz-type "interaction blocks," meaning diagrams such as (5.16) and (7.1) with no unlinked core parts and no many-body intermediate states Φ_i falling within the degenerate subspace. Arrange these blocks in a vertical column, and connect up the external valence lines between successive blocks to form an unfolded diagram as in (7.15). Now discard any diagrams which are not completely connected, (7.15) for example, and erase any completely noninteracting valence lines such as those in (7.16) and (7.18). Now draw a loop around each set of valence lines passing between successive blocks. The $(f+1)$ blocks are thus connected by f "bundles" of valence lines. [These loops are to prevent confusion between folded valence lines and downgoing

[68] I am indebted to Professor C. Bloch for suggesting some clarifications of these rules.

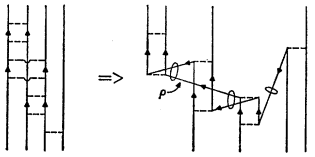
[69] The statement of the rules in Ref. 24 is incorrect with regard to the treatment of projecting core excitations.

lines representing holes in the core. Note that a diagram similar to the right-hand side of (7.18) appears also in the expansion of $\mathcal{U}_V^{(0)}$, but in that case the downgoing lines both represent holes. The downgoing lines in (7.18) are summed instead over the *valence* states, and together they carry only a *single* factor of (-1).] Finally, fold each of these "bundles" to form diagrams such as the right-hand sides of (7.16) and (7.18).

To make this last step very clear, think of drawing the diagram of the previous step on a long vertical strip of paper and then making a zig-zag fold between each successive pair of blocks. Each fold should coincide with the topmost and bottommost *valence* interactions of the neighboring blocks. [Valence interactions are those directly involving the valence particles, as contrasted to interactions in the "projecting core excitations" discussed at the end of Sec. V. All projecting core excitations factorize automatically, as explained above.]

The interactions of each block can have any relative time order with respect to those in the other blocks, subject to two restrictions: (i) *The highest valence interaction of each block must occur above the lowest valence interaction of the previous block.* Neighboring blocks must either overlap or completely overshoot each other. (ii) *The topmost valence interaction of the final folded diagram must be identical to the topmost valence interaction of the original unfolded diagram.* All diagrams satisfying these criteria must be included.

The final folded diagrams can be drawn most nearly by (a) displacing successive blocks horizontally to avoid any horizontal overlap, and (b) straightening out each folded valence line. External valence lines which pass through one or more blocks without interacting can be removed from the bundles and allowed to leave the diagram by the most direct route. A typical example consisting of four blocks ($f=3$) is shown in (7.22).



(7.22)

2. Weighting Factors

From each "exchange group" of diagrams (diagrams which transform into each other when direct matrix elements of v_{12} are replaced by exchange elements, or vice versa), select just one member (the choice can be quite arbitrary) and discard all the others. Considering all the v interactions to be "direct", replace each element $\langle ab \mid v \mid cd \rangle$ by a "direct minus exchange" element $\langle ab \mid v \mid cd-dc \rangle$. (This is now equivalent to a "dot" diagram of Hugenholtz.[29] We retain the dashed-line representation of v to avoid ambiguity of the over-all sign factor.) Now include a factor of $(\frac{1}{2})$ for each equivalent pair of lines. An equivalent pair consists of two lines which (i) both start at the same interaction, (ii) both end at the same interaction, and (iii) both go in the same direction. This rule applies to the folded valence lines *between* interaction blocks, as well as to the lines within the blocks. (It does *not* apply to the external lines.)

3. Over-All Sign Factor

It is necessary to have a consistent set of phases for the shell-model determinants Φ_i, $i \in D$. This is done by choosing a standard order for the entire set of valence orbitals. Now consider the *unfolded* diagram. Pull the *ends* of the external valence lines across each other to bring their labels into standard order. Do this at both the top and the bottom of the diagram. Now imagine placing this diagram on the front of a transparent horizontal cylinder, a glass rod for example, wrapping the external lines around the back of this cylinder, and closing the diagram by joing the ends together. Standard ordering must be observed here; the "first" line from the top must be joined to the "first" line from the bottom, etc. The sign factor is now $(-1)^{l+h+f}$, where l is the *total* number of closed loops and h is the *total* number of downgoing line segments. Closure lines count as downgoing segments, as well as holes in the core. The valence lines are all upgoing, since the diagram is in its unfolded form.

Sometimes there is a subtle problem in applying this rule. This is explained in the discussion of (B5) in Appendix B.

4. Energy Denominators

Take the *folded* diagram and "close" it as in the previous step. The closure lines each carry two labels, one from the top and one from the bottom of the original diagram. Discard the labels which came from the top of the open diagram, keeping only the *bottom* labels. [This step follows from the argument of (5.17).] The energy denominators are now given by the Goldstone prescription,

$$e_G = \sum (\text{downgoing line energies}) - \sum (\text{upgoing line energies}). \quad (7.23)$$

[Note that the folded valence line labelled ρ in (7.22) is upgoing, while the other folded lines are downgoing. The closure lines are also downgoing.]

5. Sums Over States

Within each block: Sum each upgoing line over all valence orbitals and over all the higher-lying "intermediate" orbitals. Sum each downgoing line over all core orbitals. *Between blocks*: Sum each folded line over all valence orbitals. Each summation must be done independently, i.e., without regard to exclusion, with one restriction. The many-body intermediate states Φ_i *within* each block must all be nondegenerate, thus in

each case there must be at least one particle excited out of a core orbital (thereby creating a hole) and/or at least one particle excited into an intermediate orbital. In case a degenerate state would result from two particles of an equivalent pair both occupying valence orbitals, the factor of $(\frac{1}{2})$ is to be retained if *both* of the allowed combinations "valence plus intermediate" and "intermediate plus valence" are included in the summations.

6. *Rules for Valence Holes*

A similar expansion exists for systems containing n' "valence holes" in the core, in addition to n valence particles beyond the core; $A=N+n-n'$. The valence holes are represented by n' *downgoing* external valence lines whose labels are distributed among a subset of the core orbitals called *valence hole orbitals*. The above rules are modified as follows:

Topology: Completely noninteracting valence hole lines may be ignored, otherwise no change. *Weighting factors*: No change. *Over-all sign factor*: The set of valence hole orbitals must also be given a standard order, and this must be observed when closing the diagram. The recipe is still $(-1)^{l+h+f}$, but the rule for h is different. The number of downgoing line segments must be counted *before* closing the diagram. (Example: An external hole line which interacts just once will contribute two segments.) To this number must be added the downgoing segments obtained by closing the external *particle* lines. One should note how this applies to the discussion of (B5c) in Appendix B. In that example, a reversal of all the arrows still leads to "two holes and one loop" for the double loop on the right-hand side. *Energy denominators*: No change. *Sums over states*: Within each block the downgoing lines are summed over all valence hole orbitals as well as over the remaining core orbitals. This rule is again qualified by the requirement of no degenerate intermediate states. Between blocks each folded valence hole line is summed over all valence hole orbitals.

Wave Functions and Norms

We have already discussed the adiabatic development of $\Psi=\Omega\Psi_D$ for the one-body case, as an example of the use of folded diagrams. The same description for Ψ can of course be obtained by arguments paralleling (7.2) et seq., with $\Omega_V^{(r)}$ replacing $\mathcal{U}_V^{(r)}$, Ω_V representing the $\sum_r \mathbf{Y}_r$ operator in (6.10). In the nondegenerate many-body case it was found that all "vacuum fluctuations" were eliminated by removing ΔE from the energy denominators. A similar thing happens to the valence terms in Ψ when the ΔE_V's are removed from their denominators. The valence analogs of the vacuum fluctuations (closed core parts) are pieces which look like linked parts from the BH diagrams for $\mathcal{U}_V$. The cancellation of these "closed linked valence parts" follows from the argument of (7.19)–(7.21), with only one modification. The "principal part" of an $\Omega_V\Psi_D$ diagram consists of *all* of its "open linked valence parts."

The folded diagrams which remain may still contain several linked parts, but these are all "open" in the sense that they represent excitations out of the subspace D. We denote these "folded, linked, open valence parts" by $\mathbf{Y}_{Lr}$. They are quite analogous to the $\mathbf{W}_r$'s of Sec. VI. To specify these $\mathbf{Y}_{Lr}$'s more precisely, we recall again that the "insertions" of $\mathcal{U}_V^{(r)}$ are obtained from the *reduced* BH expansion, and all projecting core excitations in these insertions must be understood to be completely factorized. The *lower* parts of the original $\mathbf{Y}_r$'s should be similarly reduced before folding in these insertions. Some further features of these $\mathbf{Y}_{Lr}$'s are discussed at the end of Sec. X.

The factorization theorem can now be applied, since the denominators no longer contain ΔE_V, and one finds that a typical diagram in Ψ has the form

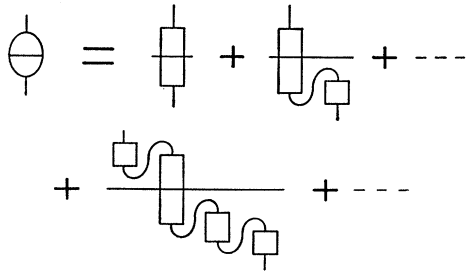
$$\left[\prod_r \frac{(\mathbf{Y}_{Lr})^{n_r}}{n_r!}\right]\left[\prod_s \frac{(\mathbf{W}_s)^{n_s}}{n_s!}\right]|\Psi_D\rangle. \tag{7.24}$$

The n_r's arise because we consider each $\mathbf{Y}_{Lr}$ to include summations over all its single-particle labels, as in (6.3). The $\mathbf{W}$'s can of course be summed into the exponential form.

For a small number of valence particles, it is more convenient to leave Ψ in terms of diagrams where exclusion is obeyed by the "incoming" valence lines, i.e., the lines entering the bottom of the set of $\mathbf{Y}_{Lr}$'s in each (7.24)-type diagram. The $\mathbf{Y}_{Lr}$'s can then be distinguished by their "incoming" labels, and all the n_r's are reduced to unity. The valence normalization factor [see (6.21)] is then just $(1-F_V')$, as before, but the diagrams will now have folded top and bottom "halves". These "halves" are the sections of the diagrams representing $\Psi^\dagger$ and Ψ, respectively. We introduce the symbol Θ to indicate the sum of all such diagrams in $(-F_V')$, thus

$$N_V=1-F_V'=1+\Theta. \tag{7.25}$$

For a simple one-body system, these Θ diagrams have the general structure shown in (7.26).



(7.26)

Their insertions and folding lines are all restricted to lie entirely above or entirely below the level (shown as a horizontal line) where the "principal parts" of Ψ and $\Psi^\dagger$ are joined together.

If there are many valence particles, the unlinked terms which remain in (7.25) and (7.26) may be troublesome. "Completely linked" expressions may be obtained by ignoring all exclusion restrictions on the incoming valence lines of (7.24). Then

$$\Omega_V = \exp\left(\sum_r \mathbf{Y}_{Lr}\right), \tag{7.27}$$

and

$$\Psi = \exp\left(\sum_r \mathbf{Y}_{Lr}\right) \exp\left(\sum_s \mathbf{W}_s\right) | \Psi_D \rangle. \tag{7.28}$$

[One need not include any individual $\mathbf{Y}_{Lr}$'s in $\sum_r \mathbf{Y}_{Lr}$ which have more than n external valence lines, since the total effect of such operators on Ψ_D must be identically zero. The resulting diagrams would all be cancelled by exchanges.] The corresponding linked valence norm is then (approximately, as qualified below)

$$N_V = \exp\left(-F_{VL}'\right), \tag{7.29}$$

where

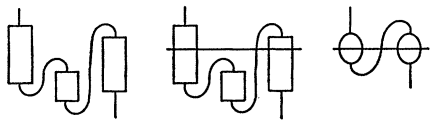
$$F_{VL} = \langle \Psi_D | \mathcal{U}_{VL} | \Psi_D \rangle = \Delta E_V, \tag{7.30}$$

and

$$F_{VL}' = \langle \Psi_D | d\mathcal{U}_{VL}/dE_0 | \Psi_D \rangle. \tag{7.31}$$

Here F_{VL} and F_{VL}' have no diagrams with more than n external valence lines, although one is free to either ignore or obey exclusion when labelling these lines.

We shall attempt to justify this exponential expression (7.29) by demonstrating its equivalence to (7.25). Consider a degenerate one-body system. Differentiation of term (a) in (7.32) will produce diagrams such as (b).



(7.32)

These are typical contributions to F_{VL} and $-F_{VL}'$, respectively. Note that (b) has *two* interaction blocks at the level where the pieces of Ψ and $\Psi^\dagger$ are joined. This really involves two of the Θ diagrams illustrated in (7.26); we represent this Θ structure by diagram (c). Using factorization and matrix-multiplication, term (b) can be viewed as a part of $-\Theta^2/2$. Continuing in this manner, we find that (minus) the E_0 derivative of the sum of the linked $\mathcal{U}_V$ diagrams, (7.31), leads to the power series development of $\ln(1+\Theta)$. The coefficient of Θ^r is now $(-1)^{r-1}/r$. The factor of $(-1)^{r-1}$ obviously arises from the folded lines between the Θ's, as in example (c) above, while the factor $(1/r)$ comes from removing a restriction originally imposed on the relative time ordering of interactions within the different Θ's in Θ^r. The topmost interaction of the Θ attached to the upper external line was originally the topmost interaction of the entire diagram. The Θ's can be factorized by relaxing this time restriction and then dividing by r to avoid overcounting. [Actually, it is more convincing to work "backwards," starting from $(\mathbf{A}_\alpha^\dagger \Theta \mathbf{A}_\alpha)^r/r$.] This confirms the (approximate) equivalence of (7.31) and (7.27) for the one-body case. The many-body case has the same topology, and the result is obviously linked.

There is another way to (approximately) verify (7.29), which also sheds some light on relations between the various kinds of diagrams. One can start with the analogous nondegenerate expression (6.4), convert the closed-loop diagrams into folded diagrams with $\leq n$ external lines, and then note that the combinatoric arguments are essentially the same for both the nondegenerate and degenerate cases.

Unfortunately, neither of these justifications of (7.29) are rigorous, and the result itself is probably inexact. The trouble is that the matrix multiplication, which is necessary for a simple linked-cluster result, is really not permissible unless Θ is diagonal in the $\mathbf{A}_\beta^{(\alpha)}$ basis. In reality, Θ is diagonalized by a very different orthogonal basis $| \chi_j \rangle$, as discussed in Appendix D, but this does not appear to be useful here. Of course (7.29) will be exact when the numbers of valence particles and valence states are just equal, since this implies that $d=1$. It should be a good approximation whenever the *complete* set of $\mathbf{A}$'s is nearly orthogonal. On the other hand, we shall obtain *exact* linked expansions for the expectation values and transition amplitudes. These are, after all, the quantities of most direct interest.

Expectation Values, Transition Amplitudes

The object here is to express the valence contributions to the transition amplitudes (6.23) in the form

$$\langle \alpha | \mathcal{O} | \beta \rangle_V \equiv \frac{\langle \Psi_\alpha | \mathcal{O} | \Psi_\beta \rangle_V}{(N_{V\alpha} N_{V\beta})^{1/2}} = \mathbf{A}_\alpha^\dagger \mathfrak{M}(\mathcal{O}) \mathbf{A}_\beta, \tag{7.33}$$

where $\mathfrak{M}(\mathcal{O})$ is a matrix consisting of linked diagrams connecting the degenerate states Φ_i. Diagrams for the individual $\mathfrak{M}_{ij}$ elements must therefore have $\leq n$ external valence lines. (In labelling these lines, one is free to either obey or disregard exclusion, provided the decision is followed consistently.) This makes it rather difficult to generalize the factorization argument of (6.8), so we shall proceed instead with the "nonexponential" forms (7.24) and (7.25).

We first consider expectation values, i.e., the diagonal terms

$$\langle \alpha | \mathcal{O} | \alpha \rangle_V = \langle \Psi_\alpha | \mathcal{O} | \Psi_\alpha \rangle_V N_{V\alpha}^{-1}. \tag{7.34}$$

By using the folded but unlinked diagrams (7.24) for Ψ, we obtain $\langle \Psi | \mathcal{O} | \Psi \rangle_V$ in terms of valence diagrams with the type of folded structure shown in (7.26). The horizontal lines in these diagrams now indicate the levels of their $\mathcal{O}$ interactions. We introduce the symbol $\odot$ for the matrix in D which these diagrams define, thus

$$\langle \Psi_\alpha | \mathcal{O} | \Psi_\alpha \rangle_V = \mathbf{A}_\alpha^\dagger \odot \mathbf{A}_\alpha. \tag{7.35}$$

Rewriting (7.25) in a similar fashion,

$$N_{V\alpha} = 1 + \mathbf{A}_\alpha^\dagger \Theta \mathbf{A}_\alpha, \tag{7.36}$$

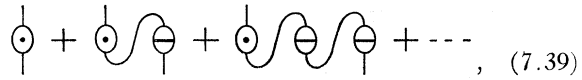
we can expand $(N_{V\alpha})^{-1}$ in a geometric series. Matrix multiplication then leads to

$$\langle\alpha \mid \mathcal{O} \mid \alpha\rangle = \sum_{r=0}^{\infty} \mathbf{A}_\alpha^\dagger \odot \mathbf{A}_\alpha (-\mathbf{A}_\alpha^\dagger \Theta \mathbf{A}_\alpha)^r = \mathbf{A}_\alpha^\dagger \mathfrak{M} \mathbf{A}_\alpha, \tag{7.37}$$

where

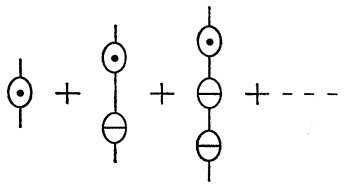
$$\mathfrak{M} = \sum_{r=0}^{\infty} \odot (-\Theta)^r. \tag{7.38}$$

The "one-body" diagrams for (7.38) are



(7.39)

or



(7.40)

in "partially unfolded" form. Note that there are no time-order restrictions between interactions belonging to different members of the set of Θ's and $\odot$. The topmost interaction in $\odot$ need not be the topmost of the entire diagram, in (7.39).

For more than one valence particle, both Θ and $\odot$ will generally have unlinked diagrams. The "folding" in (7.39) now eliminates all unlinked terms, by essentially the same argument as in (7.19) to (7.21). [The blocks in those diagrams should now be interpreted as linked parts of Θ or $\odot$. The "principal part", drawn as the upper left-hand block, now corresponds to the linked part of $\odot$ containing $\mathcal{O}$. Any other linked parts within $\odot$ will all belong now to a *single* overlapping group.] Of course there must be no exclusion restrictions on the folded valence lines between the various Θ's and $\odot$.

This expansion is complicated by the need to identify the Θ structure of each diagram, in addition to the individual folds within each Θ and $\odot$, to make sure that $\odot$ appears at the top of the partially unfolded diagrams (7.40). Except for this, and the fact that f is the total number of folds, the rules for the diagrams of $\mathfrak{M}$ are the same as for the linked expansion of $\mathcal{V}_V$. For *total* expectation values, of course, one must not forget the core term $\langle\mathcal{O}\rangle_C$ in (6.23).

We have assumed again that Θ is diagonal in the orthogonal $\mathbf{A}_\beta^{(\alpha)}$ basis, which is not strictly true. An expansion which is free of this defect, and which is obviously linked, is obtained by applying the argument of (6.10), (6.11) to the linked energy expression $\Delta E_{V\alpha} = \mathbf{A}_\alpha^\dagger \mathcal{W}_\infty \mathbf{A}_\alpha$. The result is formally exact. It differs from (7.38) in just two respects: (a) the topmost interaction of a folded diagram (7.39) is now always the same as the top of the *completely* unfolded diagram, and (b) in the partially unfolded diagrams, $\odot$ need not be above all the Θ's. In contrast to (7.38), condition (a) prevents the terms of this series from being completely factorizable into "on energy shell" Θ and $\odot$ parts. A more satisfactory exact expansion for $\mathfrak{M}$ is presented in Appendix D.

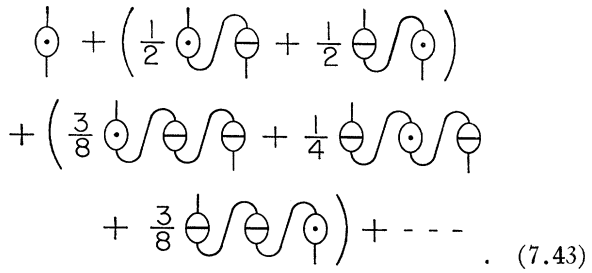
For transition amplitudes, we replace the geometric series for $(N_{V\alpha})^{-1}$ by the product of the binomial expansions[70] for $(N_{V\alpha})^{-1/2}$ and $(N_{V\beta})^{-1/2}$. We then find that (7.38) is replaced by

$$\mathfrak{M} = \sum_{r,s=0}^{\infty} \binom{-\frac{1}{2}}{r} \binom{-\frac{1}{2}}{s} \Theta^r \odot \Theta^s, \tag{7.41}$$

where the binomial coefficients for $(1+x)^{-1/2}$ are

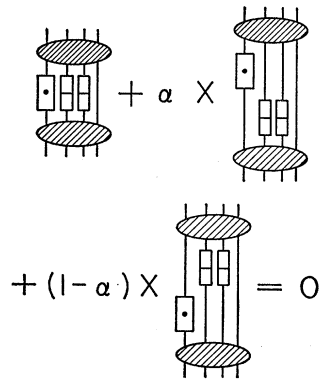
$$\binom{-\frac{1}{2}}{r} = (r!)^{-1} \prod_{i=0}^{r-1} (-\tfrac{1}{2} - i). \tag{7.42}$$

The corresponding folded diagrams are



(7.43)

There are now $(t+1)$ different Θ orderings for the diagrams with $r+s=t$. The cancellation argument of (7.19)–(7.21) still applies, as can be shown by induction: Assume that the sum of all diagrams with $r+s \leq t$ contains no unlinked terms except among the diagrams with $r+s=t$. Now consider just the "new" unlinked terms in $\Theta^r \odot \Theta^s$, i.e., those which are not cancelled by unlinked terms with $r'+s'=r+s-1$. These "new" terms can be cancelled equally well by $\Theta^{r+1} \odot \Theta^s$, or by $\Theta^r \odot \Theta^{s+1}$, or by any linear combination of these with a total weight of unity. This statement is illustrated schematically in (7.44), where α is an arbitrary parameter.



(7.44)

[70] Expansions of this type have been used in other many-body formalisms. See J. W. Clark and P. Westhaus, Ref. 23, and also P. O. Löwdin, J. Chem. Phys. **18**, 365 (1950).

The phenomenon shown in (7.21) also occurs here, and is to be handled in the same way.

We now observe that the total weight of all the $t+1$ different Θ-orderings for $r+s=t$ is the same (unity) for all values of t. From this it follows that all the "new" unlinked terms with $r+s=t$ are cancelled by terms with $r'+s'=t+1$. [Start with the "new" terms from $\odot\Theta^t$, and cancel these by adding a sufficient weight of $\Theta\odot\Theta^t$ to the amount of $\odot\Theta^{t+1}$ which occurs in (7.41). Then cancel the "new" terms in $\Theta\odot\Theta^{t-1}$ by taking the "left-over" weight of $\Theta\odot\Theta^t$, i.e., that fraction of this term from (7.41) which has not already been used up, and adding a sufficient weight of $\Theta^2\odot\Theta^{t-1}$, etc.]

The only difference between the rules for (7.38) and (7.41), apart from the different Θ ordering, is that the factor $(-1)^f$ is replaced by

$$(-1)^{f-r-s}\binom{-\frac{1}{2}}{r}\binom{-\frac{1}{2}}{s}, \tag{7.45}$$

where $(f-r-s)$ is now the number of "internal" folds within $\odot$ and Θ's.

Our derivation of (7.41) is slightly incorrect, since we have assumed again that the $\mathbf{A}_\alpha$'s are all orthogonal. Nevertheless, we find in Appendix D that this result becomes formally exact when the $\mathbf{A}_\alpha^\dagger$, $\mathbf{A}_\beta$ vectors in (7.33) are replaced by some closely related vectors $\hat{\mathbf{A}}_\alpha^\dagger$, $\hat{\mathbf{A}}_\beta$. The latter are chosen to be precisely orthogonal.

VIII. APPLICATIONS OF THE LINKED VALENCE FORMALISM

This completely linked formalism is needed whenever there are many valence particles. In rare-earth nuclei, for example, shell-model descriptions usually involve a large number of valence particles. Regardless of whether or not the ΔE_V's might be large enough to cause difficulties here, it would not be clear what to do about the many unlinked terms of the Bloch–Horowitz expansion. These difficulties can become serious in modern studies of vibrational states, where one breaks open several of the normally filled shells and excites an arbitrary number of particles out of these shells. A much more extreme example is the problem of superfluidity in nuclear matter. We shall consider both of these problems, and also some connections with Landau's theory of Fermi liquids, and with the theory of nuclear reactions.

Collective Vibrations

We begin with a rather extreme example—a "closed-shell" nucleus where all N particles are allowed to participate in collective vibrations, or in the corresponding ground-state correlations of the random-phase theory.[71] The boundary between the "valence" and the "intermediate" states, μ and b, must of course be chosen several subshells above the highest normally-filled shells. We shall see later in this section that this example is actually of considerable practical importance.

In this case there can be no "core" at all—all N particles must be regarded as valence particles. This is because the number of upgoing lines (and/or downgoing lines) at the top of a diagram must be the same as at the bottom of the diagram. (In the linked expansion this number depends on the individual diagram, but each diagram still "conserves" the number of valence particles and/or valence holes.) Thus to treat transitions across the physical Fermi surface, one must regard *all* of the coupled valence states as valence particle states, or alternatively as valence hole states; a mixture of both will not suffice.

Choosing the "particle" description here, ΔE_V becomes the *entire* interaction energy with respect to $H_0=T+V_{\mathrm{SM}}$. This is larger in magnitude than the total binding energy. (In infinite nuclear matter, this interaction energy amounts to around $+35$ or $+40$ MeV per particle.) Thus ΔE_V becomes very large, for moderate values of N, even compared to the large energy denominators (typically of order 500 MeV) appearing within the G matrices. If the Bloch–Horowitz expansion were used, this large energy shift would completely change the character of the G-matrix interactions. This makes it clear that the many unlinked terms must have a large coherent effect to compensate for this change.

The linked valence expansion demonstrates that the effective two-body interaction [the G matrix, plus the core polarization correction of (5.16c)], and the higher-order corrections to this (presumably small) are reasonably insensitive to the number of particles being treated as valence particles. This is, of course, an empirical fact, but the linked formalism is needed to prove this theoretically. One also expects that the effective interaction has *some* dependence on the choice of the model subspace. With the present formalism, this dependence can be studied in detail.[72]

This "no core" approach will have only a small effect on the shell-model potential acting on the normally occupied states, as compared to the simple closed-shell description with N core particles and no valence particles. The same self-energy processes (see Ref. 9) may be absorbed into the definition of the model potential V_{SM}, on the assumption that the valence particles are all in the simple closed-shell configuration, and all corrections to this may then be absorbed into the effective interaction $\mathcal{V}_V$. (Some refinements are suggested below.) A very important feature of this approach is that the V_{SM} acting on the "unoccupied" valence states is now essentially the same as for the normally occupied states. The discontinuity in the

[71] The ground-state correlations of O^{16} have been calculated in this way by A. Kallio [Ph.D. thesis, University of Helsinki, 1965 (unpublished)] and by G. E. Brown and C. W. Wong, Nucl. Phys. **A100**, 241 (1967). See also G. E. Brown and G. Jacob, Nucl. Phys. **42**, 177 (1963); and E. Sanderson, Phys. Letters **19**, 141 (1965).

[72] See Refs. 12, 71, and also T. T. S. Kuo and G. E. Brown, Ref. 18.

definition of V_{SM} (Ref. 9) now comes at the boundary between the "valence" and the "intermediate" orbitals. For the normally occupied states, the only change from the simple closed-shell description is that the intermediate-state summations must all correspond to many-body states outside the model subspace. In calculating the usual G matrix, for example, *both* intermediate states must be above the "ordinary" Fermi surface (due to exclusion effects from the other valence particles), and at least one of them must be outside the band of valence orbitals.

This valence particle approach is rather flexible. It also allows for the possibility of including some effects of the ground-state correlations within the definition of V_{SM}. [See (8.10) and (9.16) below.] The idea of no "core" particles may seem rather extreme, since one rarely attempts to include *all* N particles in microscopic studies of vibrations. Nevertheless, this offers a good illustration of the way the present formalism must be handled to obtain useful results. Once V_{SM} and the linked matrix elements of $\mathcal{U}_V$ have been determined in this way, the task of diagonalizing $\mathcal{U}_V$ can be handled (approximately) by the well-known "random phase" method (RPA method). This appears to require the assumption that only the one-body and two-body linked parts of $\mathcal{U}_V$ are significant. In practice one can get around this restriction, as shown in the discussion of (8.1) below.

Quasi-Particle Diagrams, Fermi Liquid Theory

Another important possibility is to treat this "reduced Hamiltonian" problem, $\mathcal{H}_D = H_{0V} + \mathcal{U}_V$, by a *second* application of linked-cluster perturbation theory. For the closed-shell nucleus we have been discussing, the diagrams can be represented most conveniently by the usual "Φ_0 vacuum" convention, where all upgoing and downgoing lines refer to departures from the normal closed-shell configuration Φ_0. Note, however, that this convention must not be introduced until *after* the linked $\mathcal{U}_V$ diagrams have been calculated by the above procedure.

These new diagrams have a very different meaning from the ones used previously. They refer only to configurations within the model subspace. Only the system's valence particle degrees of freedom are involved, and these, by analogy to the Landau theory of Fermi liquids,[73] might equally well be called the quasi-particle degrees of freedom. These new diagrams are therefore "quasi-particle diagrams."

A very important reason for doing nuclear calculations in two stages, as outlined above, is that this allows for a careful treatment of the shell structure details of the low-lying intermediate-state orbitals. This is essentially impossible in a "one-stage" treatment, since the G-matrix elements must necessarily be evaluated by using some sort of continuum approximation which smears out all the shell structure of the intermediate states. Furthermore, the weak intermediate-state potentials recommended in Refs. 9 or 11 will have already eliminated most of this shell structure anyway. Another important consideration is that the expansion may converge poorly unless the low intermediate states are handled in this way. (This is discussed below.)

So far, we have considered only the nondegenerate case of a "closed-shell" nucleus. Open-shell problems may be treated similarly, by now applying degenerate perturbation methods within the original subspace D (the *primary* subspace). Thus it is useful to make a *second* partition of the configuration space, to distinguish between "low," "medium," and "high" configurations. The first partition takes care of the very high configurations arising from the singular part of v. There is a natural small parameter here, and this part of the calculation should converge rapidly. The intermediate orbitals here are essentially plane waves. The remaining orbitals will experience a strongly attractive potential, and these will have the familiar shell structure. (For sensible choices of D, the highest of these orbitals will be unbound and will show a resonance behavior instead.) The second partition (now a partition of the primary subspace) is to separate out the "low" configurations, namely those associated with a "simple shell-model" description. This *secondary* subspace corresponds, therefore, to the usual model subspace. Its model interaction will now include renormalization effects from the "medium" configurations, with the latter treated by shell-model techniques.

This "double partitioning" method has been applied to O^{18} and several other nuclei by Kuo and Brown.[18] In their O^{18} calculation, for example, they used a primary subspace of all shells up to and including the f shell. The higher configurations were then used to renormalize their $\mathcal{U}_V$ for a very conventional model subspace of two neutrons in the $2s_{1/2}$–$1d_{5/2}$ subshells. They found a significant renormalization effect from the core polarization process shown in (5.16c), and this considerably improved the agreement with experiment.[74] The detailed shell structure of the medium configurations was essential for this result.

This program also agrees with the currently accepted picture of the effective interaction for nuclear pairing calculations. It is well established that this interaction depends sensitively on the size of the model subspace,

[73] L. D. Landau, Soviet Phys.—JETP **3**, 920 (1957); **5**, 101 (1957); and **8**, 70 (1959); A. A. Abrikosov, L. P. Gorkov, and I. E. Dzaloshinski, *Methods of Quantum Field Theory in Statistical Mechanics* (Prentice-Hall, Inc., Englewood Cliffs, N. J., 1963); R. Balian and C. DeDominicis, Nucl. Phys. **16**, 502 (1960), also in Physica **26**, S94[3] (1960), also in *Lectures on the Many-Body Problem* (Naples, 1962), E. R. Caianiello, Ed. (Academic Press Inc., New York, 1962), see also Ref. 119; A. Klein, Phys. Rev. **121**, 957 (1961), also in Ref. 92; P. Nozieres and J. M. Luttinger, Phys. Rev. **127**, 1423 and 1431 (1962); L. P. Kadanoff and G. Baym, *Quantum Statistical Mechanics* (W. A. Benjamin, Inc., New York, 1963); R. A. Craig, Ann. Phys. (N.Y.) **40**, 416, 434 (1966). The only formalisms, other than the present one, which appear capable of producing quantitative results from "first principles" are those of F. Y. Wu and E. Feenberg, Phys. Rev. **128**, 943 (1962); W. E. Massey, Phys. Rev. **151**, 153 (1966), and of E. R. Tuttle and F. Mohling, Ann. Phys. (N.Y.) **38**, 510 (1966).

[74] For a related study of renormalization effects, see N. De Takecsy, Nucl. Phys. **A95**, 505 (1966).

being strongly renormalized by the "far" pairing configurations, whereas final results are rather insensitive to the model subspace.[75] One might also attempt a similar treatment of the far configurations of the RPA coupling scheme, including them within the effective particle–hole interaction by perturbation methods, for cases where these configurations are known to have a significant effect.[76]

These methods should also work for an infinite system such as nuclear matter or liquid He^3. This should allow one to derive *and calculate* effective quasi-particle energies and interactions within a band of valence orbitals near the Fermi surface. This amounts to another formal justification for the Landau theory. In contrast to the previous formal derivations,[73] however, this approach offers the prospect of *quantitative* calculations[50] for the basic parameters. Admittedly, this approach to liquid He^3 faces severe obstacles because of the high-density nature of the system. But these problems deserve to be re-examined in the light of recent advances concerning the convergence of the Brueckner theory.

To emphasize the connections between the Fermi-liquid theory and the nuclear methods just discussed, one might say that the final valence particles (those of the secondary subspace) are the "real" quasi-particles, and the medium configurations are composed of "virtual" quasi-particles. One can also be more specific.[77] The effective two-body interaction within the *primary* subspace corresponds to Landau's $\Gamma^{(1)}$ vertex function. This should include "apparent" two-body interactions arising from primary three-body interactions, etc., as described below. The Γ^{ω} function (equivalent to the f function) corresponds to a two-body interaction within the *secondary* subspace, this being a narrow band of orbitals near the Fermi surface. One obtains Γ^{ω} from $\Gamma^{(1)}$ by an integral equation which generates ladder diagrams. Thus Γ^{ω} is quite similar to the Brueckner reaction matrix, except that: (i) the "bare" two-body interaction v is replaced by $\Gamma^{(1)}$; (ii) the two-body intermediate configurations must lie outside the secondary subspace but must remain within the primary subspace; (iii) "folded" ladders are now included. The pair of lines between successive interactions may go downwards as well as upwards; this "doubling back" is permitted as long as both members of the pair go in the same direction. To this result should be added the apparent two-body interaction terms (for the secondary subspace) arising from the three-body terms (8.1) which are generated by $\Gamma^{(1)}$ interactions acting *within* the primary subspace but *beyond* the secondary subspace. Finally, the Γ^{k} function, which determines the transport properties, corresponds to the effective particle–particle interaction used by Kuo and Brown[18] for O^{18}. This includes all of the Γ^{ω} processes, *plus* all exchanges of virtual particle–hole excitations, the simplest example of the latter being (5.16c). For these latter processes ("core polarizations") the effective particle–hole interaction is Γ^{ω}. Note that, in contrast to Green's function methods, the present approach provides a well-defined cutoff for the intermediate-state summations in the integral equations for Γ^{ω} and Γ^{k}. This is because all intermediate configurations must be within the primary subspace; it has nothing to do with the damping of "real" quasi-particles.

We should emphasize another of the important ideas of the Landau theory. Consider the linked three-body terms in $\mathcal{U}_V$, as shown in (8.1).

(8.1)

It would be very difficult to include *all* the effects of these processes in a shell-model calculation, but we need not go to the other extreme of completely ignoring them. Instead, we may take advantage of the fact that the quasi-particle occupation numbers [the $P_{\mu}^{(0)}$'s of (5.7)] are almost unity (zero) for the states below (above) the Fermi surface. Thus it is very reasonable to sum one of the external lines over all of the normally occupied states, with weight unity (all combinations of one lower line and one upper line should be considered here), and to regard the result as a *renormalization* of the effective two-body interaction. The true three-body nature of this term will then show up only through the *deviations* of the $P_{\mu}^{(0)}$ distribution, for the "third" particle, from the simple step-function form appropriate to a noninteracting system. (In case of double partitioning, these $P^{(0)}$'s should be the ones referring to the *secondary* subspace.)

Actually, we must use exactly the same type of argument to introduce the apparent one-body interaction V_{SM} in the "no core" formulation. In this case, V_{SM} arises mainly from the linked two-body cluster terms in $\mathcal{U}_V$, but V_{SM} also has important contributions from linked three-body terms (the U_3 term of Ref. 9), and from combinations of several two-body interactions (the U_{2S} term), etc. Returning to the "fundamental" three-body cluster term (8.1), we see that it contributes to the "zero-body" term (the binding energy for the simple closed-shell configuration $\Psi_D \rightarrow \Phi_0$), to the one-body interaction (V_{SM}), and to the apparent two-body interaction. It also gives rise to an *apparent* three-body interaction, but this latter effect should be quite weak. The weakness here is because this effect now involves the *third power* of the difference between the interacting and noninteracting quasi-particle distributions $P_{\mu}^{(0)}$. This weakness of the *apparent* three-

[75] See for example V. Gillet, B. Giraud, and M. Rho, Nucl. Phys. (to be published).

[76] A related proposal has been made by N. De Takecsy, Phys. Letters **23**, 260 (1966). A case where the "far" configurations are important has been studied by V. Gillet, A. M. Green, and E. A. Sanderson, Nucl. Phys. **88**, 321 (1966).

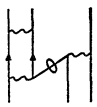
[77] Identifications of the following type were first suggested by V. J. Emery (unpublished), and are mentioned in the second paper by Kuo and Brown, Ref. 18. I am indebted to these authors, and to G. V. Chester and J. W. Kane for useful discussions.

body effects is the essential content of the statement that a Fermi liquid may be viewed as a low-density gas of weakly interacting quasi-particles.

Time-Dependent Problems

We mentioned at the end of Sec. VI that problems with a strong time dependence (nuclear reactions, for example) might be handled by the techniques of this section. In all of the developments so far (except for remarks about the Landau theory) we have been dealing with the exact eigenstates of the total system. This is not the case for time-dependent problems. The eigenvalue or "frequency" dependence of the effective interaction $\mathcal{V}_V$ may now become very important, since one is now dealing with a mixture of eigenstates. We believe that the most practical way to approach nuclear reaction problems, such as the calculation of the optical potential, is again to handle the job in two stages.

The first step is to calculate the interaction $\mathcal{V}_V$ for a model subspace large enough to include all of the usual "strong coupling" degrees of freedom. Intuitively, one expects that if the model subspace is made large enough, the denominators appearing within $\mathcal{V}_V$ [see equations (2.7), (2.12)] will all be so large that its energy dependence can, in some sense, be neglected. This comes out rather nicely in the linked formalism. Much of the energy dependence is contained already in the one-body and two-body effective interaction terms. This part can be treated essentially exactly, by (a) using self-consistent single-particle energies, and (b) by partially summing all diagrams like (7.18) which contain folded two-body insertions. The remaining energy dependence will be negligible, to the same degree of approximation as the neglect of the *apparent* many-body effective interactions. For example, a three-body effective interaction term which really arises from two-body effects is shown in (8.2).



(8.2)

This shows a two-body contribution (right-hand side) to the "frequency" dependence of the basic two-body interaction (left-hand side). Much of the effect of this term can still be treated exactly, according to the discussion of (8.1), and there are excellent reasons for neglecting the remaining "apparent" three-body effects.

For the second step, one might use a time-dependent formalism to study the evolution of the model wave function $\Psi_D(t)$ under the influence of $\mathcal{H}_D = H_{0V} + \mathcal{V}_V$. Fourier transformation would then lead to a "quasi-particle Green's function" description. In this language, the interesting frequency or energy dependence of the mass operator now arises *entirely* from the "near" configurations within the model subspace. Another practical advantage of this approach is that the H_{0V} eigenvalues (for the "noninteracting quasi-particles") are all real. But there is also a difficulty. Many of the "model" orbitals will be unbound, and must therefore lie in the continuum. A number of investigators are studying this problem in the "many-body" or "continuum shell-model" theory of nuclear reactions.[78] That theory fits very well into the present framework.

We have suggested a "quasi-particle Green's function" formalism for two reasons. The first and most obvious one is that degeneracy or strong configuration mixing may rule out perturbation treatments. This is certainly the case when pairing correlations are present. The second reason is that a *true* Green's function treatment is much too cumbersome. The *true* spectral weight function must have a very long and relatively large tail at high energies, due to effects of the hard core.[79] Serious approximations have had to be introduced in all *true* Green's function calculations to date,[80] and we do not believe that the short-range multi-particle correlations can be treated as adequately or as easily as by Brueckner-theoretic methods. The restriction to configurations within the model subspace, and especially the use of a non-singular interaction (from $\mathcal{V}_V$), should eliminate this large tail from the quasi-particle spectral weight function. In the approximation of neglecting pairing and collective mode effects, this treatment of the optical potential problem would become very similar to the perturbation-theoretic method of Hugenholtz,[29] as mentioned at the end of Sec. VI. The difference lies mainly in our specific choice

[78] See, for example, U. Fano, Phys. Rev. **124,** 1866 (1961); W. H. MacDonald, Nucl. Phys. **56,** 636 (1964); C. Bloch, *Proceedings of the International School of Physics "Enrico Fermi," Course 36* (Varenna, 1965), C. Bloch, Ed. (Academic Press Inc., New York, 1966); V. V. Balashov *et al.*, Soviet J. Nucl. Phys. **2,** 461 (1966); W. Glöckle, J. Hüfner, and H. A. Weidenmuller, Nucl. Phys. **A90,** 481 (1967); M. Bauer and F. Prats, *ibid.* **89,** 230 (1966); B. Buck and A. D. Hill, *ibid.* **A95,** 276 (1967); J. Hüfner, C. Mahaux, and H. A. Weidenmuller, Nucl. Phys. (to be published).

[79] This follows from physical considerations: If a particle is suddenly added to an interacting system, *without* any dynamical correlations between the added particle and the original system, a singular interaction will produce violent transient effects. These correspond to a rapid generation of short-range correlations between the added particle and the rest of the system. (This is the physical content, in the present case, of the process of "clothing" the bare particle.) Fourier transformation then shows that there must be strong high-frequency components in the spectral weight function. The existence of a significant high-frequency "background" (non-Lorentzian term) can also be inferred from the sum rule for the spectral weight function. It is noteworthy that none of the *true* Green's function calculations of nuclear matter (Ref. 80) have taken proper account of this important feature. This neglects a large fraction of the *true* kinetic energy, as discussed in Ref. 9, and it also leads to a serious violation of particle conservation. It should be possible to refine the approximations to remedy these serious defects, but we believe that the result would then be far more cumbersome than the use of Brueckner-theoretic methods.

[80] 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); D. E. Beck and A. M. Sessler, Phys. Rev. **146,** 161 (1966).

of partial summations, and especially our single-particle energies (see below).

Superfluidity

We shall now argue that the present linked expansion provides a rigorous and completely nonsingular method for studying superfluidity in infinite nuclear matter. This is a rather academic problem, but it has long been considered a serious stumbling block for nuclear matter theory. The program consists of three quite independent steps: (i) The elimination of unlinked terms by means of the present expansion, followed by upgoing ladder summations to express this in terms of G-matrices. (ii) A study of the higher-order diagrams, to determine the validity of the usual assumption that the only important terms in $\mathcal{U}_V$ are the effective two-body interactions. (iii) Approximate diagonalization of the reduced Hamiltonian. The methods of superconductivity theory, including the Bogolubov–Valatin transformation, need not be introduced until this last step. In contrast to other formalisms that have been suggested for this problem,[81] this one distinguishes quite clearly between these basically different types of difficulties. It also permits the approximations in (ii) and (iii) to be refined separately.

In applying the present formalism here, the main problem is to organize the partial summations to make sure that the treatment is completely free of singularities. We shall base this discussion on a "large core" formulation which differs somewhat from the previous "no core" approach. This new approach is not absolutely essential here, but it seems more natural for the present problem.

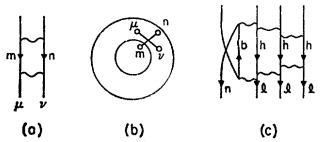
The "normal core" can be made free of singularities by (a) starting out with a "large" core, that is, by choosing the boundary between the core and the intermediate states to lie above the normal Fermi surface, at the *top* of the band of strongly coupled valence states, and (b) by using the "on-energy-shell" self-energies of Ref. 9. This leads to an artificial gap in the spectrum of *unperturbed* single-particle energies. This gap occurs at the "large" Fermi surface, and it completely eliminates the problem of small energy denominators for the "core" part of the calculation. (The magnitude of this gap is quite large. It can be reduced somewhat, with some improvement in the rate of convergence, by using the intermediate-state potentials advocated by Bethe. See Fig. 1 below. For a realistic calculation, it would probably be necessary to use a "double partitioning" treatment to deal adequately with the low intermediate states. We ignore this complication here.)

The strongly coupled states must now be treated as *valence hole* states, since the core has been chosen to be too large. After the matrix elements of $\mathcal{U}_V$ have been calculated by this procedure, one may then re-express the results in the more conventional language of particles and holes near the normal Fermi surface. The width of the valence band, energy wise, must of course be chosen to be somewhat greater than the resulting BCS gap parameter.

In evaluating the self-energy insertions, better overall convergence will be obtained by summing the internal downgoing lines (those within the insertions) only over the states in the *normal* Fermi sea. Then, as far as the "normal core" is concerned, there are only two slight differences from the treatment of normal (nonsuperfluid) nuclear matter. (1) Transitions from states below the normal k_F to states just above this k_F are now forbidden by the "large core" exclusion operator. These processes are included instead within the effective interaction $\mathcal{U}_V$. (2) As shown below, the single-particle energies of the states within the valence band must be somewhat different from those of the other core states. These changes are important mainly for $\mathcal{U}_V$. Thanks to the large gap in the single-particle energies, neither of these changes can have much effect on the "core" part of the calculation.

Elimination of $\mathcal{U}_V$ Singularities

There still remains the problem of guaranteeing that the prescription for $\mathcal{U}_V$ is free of singularities. Situations which are apt to cause trouble are shown in (8.3).



(8.3)

In (a), we see two external holes dropping down into core states below the valence band. Suppose the single-particle energy spectrum were continuous at the bottom of the valence band. Then for two external holes just at the bottom of the valence band, the energy denominators could become arbitrarily small. This could easily give rise to the type of ladder-sum divergence familiar in previous versions of nuclear matter theory. Worse still, there are also cases where only *one* of the states m, n (let us say m) is below the valence band. This would not be a problem if the valence states were strictly degenerate. But for the more interesting case of quasi-degeneracy, there is now the possibility that the hole n may have a *higher* energy than the original external valence hole. This could easily lead to vanishing energy denominators. An example of this possibility, which is consistent with momentum conservation, is shown in (b). This is a diagram in momentum

[81] A general review of methods for treating superfluid effects in nuclear matter has been given by J. S. Bell, Ref. 20. See also V. J. Emery, Nucl. Phys. **12**, 69 (1959); and **19**, 154 (1960); A. Katz, *ibid.* **18**, 177 (1960); E. M. Henley and L. Wilets, Phys. Rev. **133**, B1118 (1964); R. Kennedy, L. Wilets, and E. M. Henley, *ibid.* **133**, B1131 (1964). For a good physical discussion with a minimum of mathematics, see E. Jakeman and S. A. Moszkowski, Phys. Rev. **141**, 933 (1966).

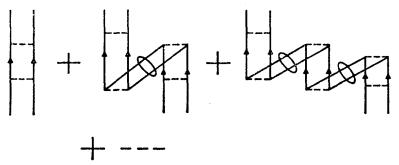
space—the concentric circles represent the boundaries of the band of valence states. A similar problem can arise in cases where a few particles (say only one) are excited from near the top of the valence band to a low-lying intermediate state b, at the same time that many valence particles drop from the top to the bottom of the valence band. An example is shown in (c), where b is a low-lying intermediate state, and "h" and "l" indicate states "high" and "low" in the valence band. The gap in the single-particle spectrum will prevent vanishing energy denominators unless a large number of valence particles (or holes) act coherently, as they do in (c). Fortunately, case (c) can never be important in practice because of the large magnitude of the gap.

These embarrassing singularities are the result of two circumstances. In the first place, the present formalism was derived under the assumption of *exact* degeneracy, and then "analytically continued" to the case of quasi-degeneracy. From the latter standpoint, the choice of the subspace D has only the virtue of descriptive convenience. It unfortunately does not guarantee that the "nondegenerate" many-body states Φ_i will all have higher energies than the "quasi-degenerate" Φ_i's. Secondly, we have removed the valence interaction energy ΔE_V from the energy denominators. This was necessary for the elimination of unlinked terms, and also because ΔE_V is proportional to the size of the system (in the superfluidity problem). But the situation is not all bad, since D presumably contains *all* of the low configurations which are strongly coupled in the ground and low-lying states. It should not matter much if the *highest* configurations in D lie above some of the lowest "intermediate" configurations, if D has been chosen sensibly in the first place.

To eliminate these (presumably weak) singularities, we note that the folded-in insertions can be used to re-introduce a "linked part" of ΔE_V back into the energy denominators. Let ΔE_{Vx} denote the part of the valence interaction energy arising from all linked folded x-body diagrams which share the same "conserved" quantum numbers (total momentum, for example). (This x indicates the number of *external* lines.) Then the sum of all linked x-body skeletons $\mathcal{U}_{Vx}^{(0)}$, together with all folded-in insertions of the same form, can be combined to give an equation analogous to (5.13),

$$[H_{0V}+\mathcal{U}_{Vx}(E_{Vx})-E_{Vx}\mathbf{I}_x]\mathbf{A}_x=0, \tag{8.4}$$

by reversing the argument (7.2)–(7.8). Here $\mathbf{I}_x$ and $\mathbf{A}_x$ refer only to the x-body subspace of the "folded bundles" of valence lines. For $x=2$, this procedure sums up diagrams like those in (8.5).



(8.5)

The eigenvalue

$$E_{Vx}=\mathbf{A}_x^\dagger(H_{0V}+\mathcal{U}_{Vx})\mathbf{A}_x$$
$$=E_{0Vx}+\Delta E_{Vx} \tag{8.6}$$

now enters all of the valence energy denominators in the same manner as in (5.23). Generally speaking, the auxiliary eigenvectors $\mathbf{A}_x$ will have no physical significance. The object is simply to obtain a matrix $\mathcal{U}_{Vx}(E_{Vx})$ whose elements are all nonsingular. These matrix elements may then be used in the "real" secular equation.

Will this really eliminate the singularities? Consider a case with just one "dangerous" intermediate configuration whose energy E_1 is only slightly greater than the energy E_0 of the highest configuration in D. (We refer only to linked x-body configurations sharing the same conserved quantum numbers.) Then the skeleton diagrams with just one "dangerous" denominator, such as the first term in (8.5), will give a large *negative* contribution to ΔE. Inserting this ΔE in the denominators will then stabilize the situation, and the final ΔE will be well-behaved. This situation corresponds to the two-level model of (9.6). From this, we observe that the ground-state solution remains well-behaved even for the case $E_1<E_0$, which is pathological from the perturbation standpoint. Now consider a more realistic model having four states, with Φ_0, Φ_1, and Φ_2 in D, and with $E_0<E_1<E_3<E_2$. For relatively weak interactions V, the eigenvalues should lie close to the unperturbed energies. Then, for the *lowest two* eigenvalues, $E\approx E_0$ and $E\approx E_1$, $\mathcal{U}(E)$ will be well-behaved and the inversion $E_3<E_2$ will cause no trouble. But $\mathcal{U}(E)$ will behave "pathologically" for the remaining eigenvalues $E\approx E_3$ and $E\approx E_2$. We conclude that this procedure should work well for these eigenstates for which D is sensible, that is, when D contains all of the low and strongly coupled configurations.

Of course there will always be other eigenstates (generally of higher energy) for which this condition breaks down. A concrete example of this situation is seen in the effective particle–particle interaction, Γ^k, of the Fermi-liquid theory. (See discussion above.) This contains instabilities of the type just mentioned, arising from the excitation of particle–hole correlations ("collective modes"). The difficulty arises because of a D which includes only valence *particles*. It can be cured by enlarging D to include "real" particle–hole pairs, as in our discussion of the RPA method below.

In practice, we believe that one should always use the $\mathcal{U}_{Vx}(E_{Vx})$ corresponding to the *lowest* eigenvalue of (8.4). [Higher states of (8.4) probably relate to total eigenstates for which the D is inappropriate, as in the examples above.] We regard this procedure mainly as an existence proof, that the singularities *can* be avoided. It should usually be sufficient to approximate (8.4) rather crudely, or even to simply estimate the lowest E_{Vx} to be somewhat below the energy of the lowest

"dangerous" x-body configuration. After all, these singularities are associated only with the *highest* configurations in D, and these, presumably, are not of crucial importance for low eigenstates of the total system.

Single-Particle Energies

We now consider the choice of self-energy insertions most likely to produce a convenient and rapidly converging approximation scheme. For states *below* the valence band, it is most useful to define the self-energies in terms of the "on-energy-shell mass operator" M^{on}, as discussed in Ref. 9. For the states *within* this band, however, it will be much more convenient to use the *complete* mass operator (with certain qualifications given below).

This makes good sense physically, since one is accustomed to using "experimental" single-particle energies in shell-model calculations, as well as in the Landau theory. Ordinarily, the complete mass operator would lead to complex eigenvalues. This does not happen here because of the restriction to "nondegenerate" intermediate states, and also because of the gap between the valence and intermediate single-particle energies. Thus the energy-conserving processes (all of them, hopefully, and surely all of the physically important ones) are confined within the model subspace. (Singularities can always be cured by the method above.) This agrees with the standard shell-model philosophy, where one deals as far as possible with *real* single-particle energies.

The most important "extra" term which should be included in the valence-state energies is shown in (8.7).

(8.7)

The internal downgoing lines here should be summed over all normally occupied states. The potential energy contribution of this diagram is real and repulsive, of order several MeV. (Previous numerical results[82] for this diagram do not apply here, because of our different choice of intermediate-state energies.)

An important effect of including this term will be to introduce a *second* gap in the single-particle spectrum, at the *bottom* of the valence band. The resulting potential energy spectrum is shown in Fig. 1. This gap alone should eliminate the type of singularities shown in (a) and (b) of (8.3), if the width (k_2-k_1) of the valence band is small enough. The magnitude of the gap Δ_1 is of the order of several MeV, which should be quite sufficient for a nonsingular treatment of superfluidity. For other applications, however, the general method (8.4) may be necessary.

Another effect of (8.7) will be to alter the "effective mass" for the valence particles. In nuclear matter, the (unobservable) effective mass for the core states is well-known to be only of order $\frac{2}{3}$, i.e., $M^*/M\approx\frac{2}{3}$. On the other hand, the experimental effective mass for valence particles, as deduced from stripping and pickup reactions for example, is close to unity, and perhaps even greater than unity.[83]

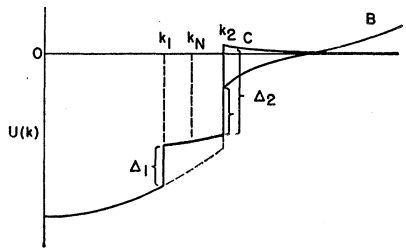


FIG. 1. Potential energy spectrum in the "large core" formulation. The limits of the valence band are at k_1 and k_2, while k_N indicates the "normal" Fermi surface. The magnitude of the gap Δ_1 has been greatly exaggerated. Note the different effective masses above and below k_1. Curve B shows the Bethe intermediate-state spectrum, Ref. 11. Curve C is the spectrum of Ref. 9.

As shown in Ref. 9, the "complete" or "field-theoretic" mass operator M^{FT} can be uniquely decomposed into on- and off-energy-shell parts,

$$M^{\text{FT}}=M^{\text{on}}+M^{\text{off}}, \tag{8.8}$$

in the context of the nondegenerate Goldstone expansion. In the present case we are using a slightly different decomposition,

$$M^{\text{FT}}=M^{\text{on},Q}+M^{\text{off},Q}+M^{D}, \tag{8.9}$$

where all the intermediate configurations within $M^{\text{on},Q}$ and $M^{\text{off},Q}$ are required (by the projection operator Q) to lie outside the model subspace D. This has only a minor effect on M^{on}, thus $M^{\text{on},Q}\approx M^{\text{on}}$. But $M^{\text{off},Q}$ is now quite different from M^{off}, since it no longer contains energy-conserving processes. The latter are (hopefully) all confined within M^{D}. This guarantees that the present valence-state energies, based on

$$M_{\text{valence}}=M^{Q}=M^{\text{on},Q}+M^{\text{off},Q}, \tag{8.10}$$

will all be real. Stated somewhat differently, we now have a Hermitian H_{0V} for the "noninteracting quasiparticles." The symbol M^{D} represents all contributions to the experimental single-particle energy arising from processes within the model subspace.

The *differences* between the unperturbed single-particle energies (E_m or E_μ) and the experimental removal energies are termed the rearrangement energies.[84] These rearrangement energies are generally

[82] K. A. Brueckner, J. L. Gammel, and J. T. Kubis, Phys. Rev. **118**, 1438 (1960); H. S. Köhler, Phys. Rev. **137**, B1145 (1965).

[83] G. E. Brown, J. H. Gunn, and P. Gould, Nucl. Phys. **46**, 598 (1963); B. L. Cohen, Phys. Rev. **130**, 227 (1963).

[84] K. A. Brueckner, Phys. Rev. **97**, 1353 (1955); N. M. Hugenholtz and L. Van Hove, Physica **24**, 363 (1958); 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).

complex (or worse, in the sense that they should really be represented by spectral weight functions). The definition of a rearrangement energy is inherently ambiguous, or model dependent, since it refers to the definition of the unperturbed energy. In our present scheme, the core-state rearrangement energies are given by

$$M_{\text{core}}^{\text{Rear.}}=M^{\text{off},Q}+M^{D}, \tag{8.11}$$

whereas the valence-state rearrangement energies are given by

$$M_{\text{valence}}^{\text{Rear.}}=M^{D}. \tag{8.12}$$

For the simple nondegenerate treatment of Ref. 9, the definition would instead be

$$M^{\text{Rear.}}=M^{\text{off}}. \tag{8.13}$$

(These expressions are only symbolic, since they define a complicated self-consistency problem. The energy shifts resulting from the M^{off} terms will also have a weak influence on the numerical values of the M^{on} terms.) Thus (8.7) may or may not be a true rearrangement energy term, depending on the context. The expression "rearrangement energy" has been used in the literature to indicate a number of different things. We would rather avoid this expression as far as possible, since it tends to cause confusion.

The main conclusion to be drawn here is that our valence state energies (8.10) are still somewhat different from the experimental energies, due to interactions with the other valence particles, although this difference may well be small. The "effective mass" may also be different. To pursue this matter further, one must also take account of the method of analyzing the experimental data to obtain real numbers for the single-particle energies. To some extent, the "experimental" single-particle energies are also model-dependent.[85] A very clear example of this is seen in the problem of nuclear pairing.[75]

Closed-Shell Systems

We return to the first problem discussed in this section, the ground-state correlations in a closed-shell system. In a finite nucleus (O^{16}) it was found by explicit calculation[12] that individual "ring" diagrams were uncomfortably large, and their sum did not appear to be converging rapidly. This led Brown and Wong[71] to evaluate *all* of the ring diagrams in closed form, using an RPA technique. This treatment was found to increase the O^{16} binding energy by roughly 1 MeV per particle, as compared to a "simple closed-shell" treatment (Ref. 9) in which all the intermediate states are regarded as being essentially plane wave states. [They are not *pure* plane waves because the latter are not orthogonal to the occupied orbitals.] This result is especially significant in view of the low binding energies found in recent calculations of finite nuclei,[7,12,13] and also for infinite nuclear matter.

Brown and Wong argued that ring correlations are quantitatively more important than Brueckner ladder correlations, for the low intermediate states, at least in finite nuclei. There, there is clear experimental evidence for the importance of rings, namely collective oscillations with enhanced transition amplitudes. They remarked, however, that the first- and second-order terms are identical in both types of summations. Thus the "rings" restore the second-order terms excluded from the G matrices by the enlarged exclusion operator $(1-Q)$ for the primary subspace.

The question arises as to whether the difference in binding energy is simply a matter of "rings versus ladders." We think not. The main point, we believe, is that their low intermediate orbitals were defined in an attractive potential well. This greatly reduced the energy denominators for transitions into these orbitals. Much of the gain in binding energy should therefore be attributed to a "spectral correction" effect, in the language of BBP. This "spectral" effect is quite significant, mainly because of the tensor force which induces strong transitions into these low orbitals. As for the "ring" and "ladder" terms beyond second order, it seems likely that they are *both* significant, and that one really ought to include both types of terms. This refinement might well be significant for the total binding energy.

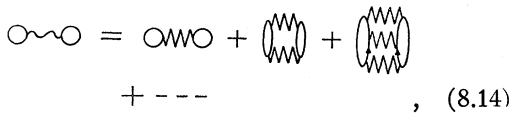
There is further evidence that this is so. We have shown previously that the "compact cluster" arrangement of the Goldstone series, which leads to negligibly small intermediate-state potentials, is the optimum way to handle the high intermediate states. On the other hand, it was clear that this procedure is unrealistic for the low intermediate states. For these, Rajaraman[86] has demonstrated the importance of repeated "bubble" insertions. (Repeated insertions are more important for low intermediate states because of the generally smaller energy denominators within the "skeletons".)

The linked valence expansion can provide (or at least suggest) more systematic ways to satisfy these conflicting requirements. Thus one can first define a primary subspace to distinguish between "low" and "high" intermediate states. All configurations beyond this subspace are to be treated by the compact-cluster scheme. One then applies the Goldstone expansion *within* the primary subspace. The two-body interactions for this expansion are G matrices defined by the enlarged exclusion operator. [This allows one of the two intermediate states to be "low", but not both of them.] Then the usual G-matrix term is represented by the

[85] J. Blomquist and S. Wahlborn, Arkiv Fysik **16**, 545 (1960); B. L. Cohen and R. E. Price, Phys. Rev. **121**, 1441 (1961); L. S. Kisslinger and R. A. Sorensen, Rev. Mod. Phys. **35**, 853 (1963).

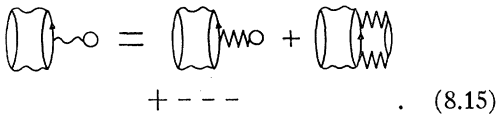
[86] R. Rajaraman, Phys. Rev. **155**, 1105 (1967).

following "quasi-particle" diagrams,



(8.14)

the sawtooth lines representing G's with the new exclusion operator. Breaking open a hole line in each of these terms, we obtain the self-energies appropriate for the hole states. These are seen to be identical, even with regard to internal-line summations, to the M^{on} insertions of Ref. 9. For *particle* states, however, we find the old off-energy-shell problem reappearing, thus



(8.15)

It appears that this effect must be treated in some average manner, as in the older treatments,[1,48] in order to obtain "potential energies" for these state.

The net result is a potential energy spectrum very similar to that of the Brueckner–Gammel calculation[1]; zero for large k's, attractive for low intermediate k's, and with a *small* jump at k_F. The diagrams of (8.14) can be calculated all at once, simply by solving the usual Bethe–Goldstone equation with this new spectrum. [Note that the third-order term in (8.14) may be significant. It should not be overlooked if the attractive part of the spectrum is treated by the reference-spectrum perturbation method. A geometric series approximation should work well, however.] To calculate the ring diagrams, the method of Gell-Mann and Brueckner might be useful, since this allows one to explicitly remove the first- and second-order terms [included already in (8.14)] before the final integration.

This whole procedure contains a "free parameter," namely the cutoff momentum k^* which defines the subspace D. One may well ask if the binding energy could be increased arbitrarily, simply by increasing this k^*. The answer is no, because an increase of k^* also enhances the off-energy-shell effects within D. Further examination leads to the conclusion, perhaps already obvious, that the explicit use of Bloch–Horowitz techniques is really unnecessary here. The same results can always be obtained by selective summations of the original Goldstone expansion, as demonstrated in (8.14).

Thus there are really two essential questions. The first is just the perennial problem of finding a proper choice for the intermediate-state potentials. Secondly, it is important to know whether the higher-order ring terms (or any other diagram sequences which depart from the compact-cluster scheme) are significant enough, for the states near the Fermi surface, to deserve a special treatment. Brown has suggested,[87] for example, that rings might be quite significant in liquid He^3, because of the large spin-wave fluctuations. (Superfluid correlations are another example, but their effect on the total binding energy is quite negligible.)

These questions cannot be decided by purely formal arguments. One's strategy here must be based on a detailed knowledge of the relative magnitudes of the various contributions, and more exploratory calculations may be necessary. In any event, we believe that the following considerations are and will remain valid. (1) An expansion in powers of κ is appropriate for the short-range part of the interaction v. (2) This ordering of the expansion is *not* appropriate for the long-range part of the potential, as Bethe has suspected and as Rajaraman has now clearly demonstrated. (3) For correlations near the Fermi surface, one expects and would like to have a potential function which is continuous (or nearly continuous, at least) near k_F. This is necessary for a realistic treatment of any "special" correlations (rings, for example) near the Fermi surface. (This is clearly essential also for a study of excited states. But there is no *a priori* reason that the "best" scheme for calculating the ground-state energy should agree with the "best" scheme for excitations.) (4) The derivative of the G matrix with respect to changes in the single-particle potentials is essentially κ. Indeed, this is the way κ was defined in Ref. 9. The complete expansion remains well-defined for any reasonable potential spectrum, and all of the "spectral corrections" can be ordered in powers of κ.

Putting this all together, we suggest that one should define the potentials for the low intermediate states ($k \lesssim 2k_F$, say) using the *same* insertions as are used for the occupied states, with the off-energy-shell effects included in some average manner. (Some of Bethe's core-suppression effect might also be included here.) The details of this averaging must depend on the relative magnitudes of the various types of correlations, since the off-energy-shell effect varies from term to term. A general requirement, however, is that the intermediate spectrum should be continuous (or nearly so) at k_F. The high intermediate states are best left with zero potential. Such a spectrum is necessarily a compromise. Nevertheless, it has the virtue of including the long-range parts of v to all orders, for the low intermediate states, in agreement with Rajaraman's proposal. Finally, we note that all remaining corrections to this "averaged" treatment of the off-energy-shell problem may then be expanded in powers of κ, in parallel with the compact-cluster expansion for the high-momentum components.

What about Rajaraman's previous suggestion[88] of regarding the third-order ring diagram as a statistical-

[87] G. E. Brown (private communication).
[88] R. Rajaraman, Phys. Rev. **129**, 265 (1963).

weight correction to the third-order "bubble" diagram? This is a convenient trick, and it should probably be used for the high intermediate states within the three-body clusters. But this is undesirable for the low intermediate states, because (a) it would produce an unphysical discontinuity in the potential spectrum at k_F, and (b) because if the ring is really significant for the low intermediate states, it should be grouped together with the higher-order rings.

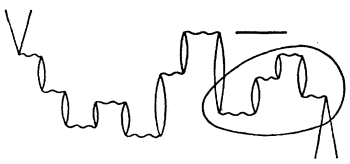
One can argue intuitively that a particle "feels" the long-range attraction of many other particles, whereas the short-range repulsion can only be communicated by a few particles. On this basis Rajaraman suggested that the interaction v should be "separated" in coordinate space, as in the Moszkowski–Scott method. For the higher-order diagrams this leads to uncontrollable approximations. One can accomplish essentially the same thing by performing a separation in momentum space. The linked valence expansion demonstrates that this can be done in a fully systematic way.

These comments are far from being a "solution" of the problem. But we hope that they shed some light on the diversity of proposals that have been made recently. An attractive intermediate-state potential will surely increase the binding energy, and this appears desirable at the present time. Nevertheless, one should not minimize the possible importance of relativistic effects, special mesonic effects, etc. We are only trying to clarify the nature of the remaining uncertainties in the "ordinary" many-body problem.

Random-Phase Approximation

It may be of interest to see how the random phase approximation emerges from the present formalism. We consider a closed-shell nucleus, and we assume that a "real" particle–hole pair has somehow been created. A secondary subspace is then defined to contain all one-particle–one-hole configurations within certain shells near the Fermi surface. The object now is to find the interaction energy, $\Delta E_V = \Delta E_{\rm ph}$, of this "real" particle–hole pair. As usual, this pair is coupled to the virtual particle–hole pairs which exist already within the true ground state.

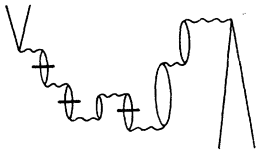
We begin with the Bloch–Horowitz expansion, a typical diagram of which is shown in (8.16).



(8.16)

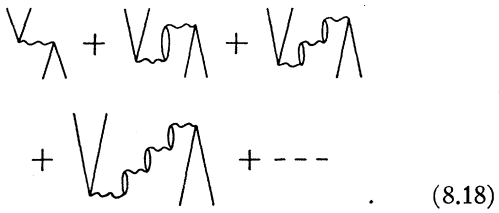
The wiggly lines here now represent the effective two-body interactions appropriate for the present problem (the Γ^ω terms discussed above). We now identify the *highest* interaction in (8.16); this is indicated by the horizontal line. Expanding ΔE_V out of the denominators, we find that (8.16) is cancelled by a similar folded diagram. In general, the folded expansion will have no diagrams with interactions connected between the *highest* interaction and the *bottom* pair of external lines. The interactions removed by "folding" are encircled in (8.16).

We note, now, that the remaining diagrams all have the structure of a set of skeleton processes together with repeated insertions, including "higher-generation" insertions, etc. The surviving portion of (8.16) is redrawn in (8.17), with the boundaries between the various irreducible parts indicated by horizontal bars.



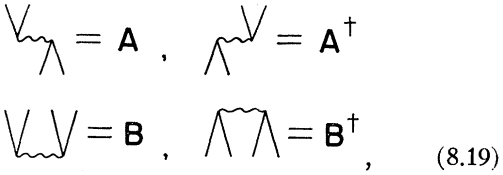
(8.17)

The general form of these irreducible parts is:



(8.18)

Except for the first-order term, these all consist of a single "backward going" string of bubbles. We shall follow Thouless' notation,



(8.19)

to express this result algebraically. The renormalized interaction for the one-particle–one-hole subspace is therefore

$$\begin{aligned}\mathcal{V}_{\rm ph}(\Delta E_{\rm ph}) &= \mathbf{A}+\mathbf{B}[-2E_{\rm ph}{}^0-\Delta E_{\rm ph}]^{-1}\mathbf{B}^\dagger \\ &\quad +\mathbf{B}[-2E_{\rm ph}{}^0-\Delta E_{\rm ph}]^{-1} \\ &\quad \times\mathbf{A}^\dagger[-2E_{\rm ph}{}^0-\Delta E_{\rm ph}]^{-1}\mathbf{B}^\dagger+\cdots \\ &= \mathbf{A}-\mathbf{B}[2E_{\rm ph}{}^0+\Delta E_{\rm ph}+\mathbf{A}^\dagger]^{-1}\mathbf{B}^\dagger, \end{aligned} \tag{8.20}$$

where

$$E_{\rm ph}{}^0 = E_{\rm p}{}^0 - E_{\rm h}{}^0$$

is the unperturbed energy of the pairs (calculated within the primary subspace). Introducing

$$\hbar\omega_{\rm RPA} \equiv E_{\rm ph} = E_{\rm ph}{}^0 + \Delta E_{\rm ph}, \tag{8.21}$$

the model secular equation now becomes

$$[H_{\rm ph}{}^0+\mathbf{A}-\mathbf{B}(H_{\rm ph}{}^0+\mathbf{A}^\dagger+\hbar\omega)^{-1}\mathbf{B}^\dagger-\hbar\omega]\mathbf{X}=0, \quad (8.22)$$

where we have identified the one-particle–one-hole state vector $\mathbf{A}_{\rm ph}$ with the "**X**" vector of nuclear RPA calculations. [We have assumed exact degeneracy of $H_{\rm ph}{}^0$ and then used (5.17).] Then by introducing

$$\mathbf{Y}=-(H_{\rm ph}{}^0+\mathbf{A}^\dagger+\hbar\omega)^{-1}\mathbf{B}^\dagger\mathbf{X}, \quad (8.23)$$

we recover the familiar result

$$\begin{pmatrix}(H_{\rm ph}{}^0+\mathbf{A}) & \mathbf{B}\\ -\mathbf{B}^\dagger & -(H_{\rm ph}{}^0+\mathbf{A}^\dagger)\end{pmatrix}\begin{pmatrix}\mathbf{X}\\ \mathbf{Y}\end{pmatrix}=\hbar\omega_{\rm RPA}\begin{pmatrix}\mathbf{X}\\ \mathbf{Y}\end{pmatrix}. \quad (8.24)$$

There is an interesting technical point in this development, namely, the unexpected sign change for the $\Delta E_{\rm ph}$ term in the energy denominators. The original valence denominators (5.23) contain $+\Delta E_{\rm ph}$. However, the BH diagrams (8.16) are seen to consist of a single skeleton part with *two* strings of insertions, one string being attached to each end of the skeleton. Each of these strings is found to contribute $-\Delta E_{\rm ph}$ to the skeleton energy denominators, leaving a net result of $-\Delta E_{\rm ph}$. A similar sign change is found in studying the contribution of on-energy-shell insertions, $M^{\rm on}$, to the self-energy of a single valence particle. [Compare this with the discussion below (5.21).]

Vertex Renormalization

One of the interesting features of the microscopic theory of Fermi liquids, as deduced from the Green's function formalism, is the renormalization of the external lines of the "vertex function." In the RPA example just discussed, the vertex function for "real" particle–hole interactions (in the subspace of a single particle–hole pair) consists of the skeleton diagrams of (8.18). For a particle–particle subspace, as in the O^{18} calculation of Kuo and Brown, the vertex function consists mainly of the terms (a) and (c) of (5.16). In other words, the vertex function amounts to the linked $\mathcal{V}_V$ pieces for the *secondary* subspace. The "irreducible" vertex function then corresponds to the two-body effective interactions of the *primary* subspace, such as the **A**'s and **B**'s in (8.19). Green's function methods have produced the result that each of the four external lines of the irreducible vertex function should be multiplied by a renormalization factor of $Z^{1/2}$, where Z (or a, in the Russian literature) is the strength of the quasi-particle pole for the one-body Green's function. By construction, a similar result obtains for the "complete" or "reducible" vertex function. We shall obtain very similar results by summing diagrams. The results are not identical, however, and we believe that the difference is physically significant.

Consider the "bare" particle–hole interaction **A** of (8.19). In addition to this, the BH expansion for $\mathcal{V}_{\rm ph}$ is found to contain the terms shown in (8.25).

(8.25)

These are all $f=0$ terms, in the language of Sec. VII. It is easily seen that term (a) is eliminated from the folded expansion, by an $f=1$ term of similar form. Terms (b) and (c) remain in the folded expansion. Term (b) represents the original vertex multiplied by M', the derivative of the $M^{\rm on}$ self-energy operator of Ref. 9. Term (c) contains two of these M' factors. These are the leading terms in the expansion of $(1-M')^{-1}$. The latter expression was shown in Ref. 9 to have a very simple physical interpretation [see also (9.9) below]. For a normally occupied state this factor gives the occupation probability P_m, and for a normally occupied state it gives the "emptiness probability" $(1-P_b)$. These P's refer to the occupation probabilities for the true interacting ground state, *before* the creation of the "real" particle–hole pair. The essential features are illustrated in Fig. 2 below.

Of course there are also diagrams in which *both* of the lower external lines carry an arbitrary number of these M' insertions. (All such insertions in the *upper* external lines are removed by "folding".) Thus both of the lower lines are renormalized in this manner, the hole (particle) line according to the true occupation (emptiness) probability of the orbital, as calculated for the interacting ground state in the absence of the valence particles. A similar result applies for the "bare" particle–particle vertex (5.16a), where the lower particle lines both acquire "emptiness' factors.

These results are very intuitive—just what one would expect for the exclusion effect of correlations within the closed-shell core. They agree also with the propagator renormalization scheme of Ref. 9. It was mentioned there that every *internal* line of a BH diagram can be "dressed" with M' insertions to produce weighting factors of P_m or $(1-P_b)$. The same applies for the folded diagrams. One would arrive at the same result by taking renormalized "irreducible vertices" and connecting them together to form a complete diagram for $\mathcal{V}_V$. But this last argument is only a consistency check. The correct procedure is to deal directly with the folded expansion, dressing the internal and *lower* external lines by straightforward summations of M' insertions.

Three points deserve further comment. First, one will note that the result is not Hermitian because of the obvious lack of symmetry; only the *lower* external lines have been renormalized. This is an inherent property of the whole Bloch–Horowitz formalism; it

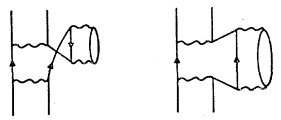
originates in the "model description" [see (2.9), (2.10), and (9.20)], whereby one calculates the *projections* of the complete wave functions on the model subspace. These projections need not be orthogonal. (One knows, for example, that the "**X**" vectors of the RPA method are not orthogonal.)

For some purposes, however, one might want a Hermitian interaction operator. This is provided, as explained in Appendix D, by the "natural transformation" (D35). We need simply remark that the linked one-body parts of the $(1+\Theta)$ operator will include the *entire* geometric series $(1-M')^{-1}$. It follows that *all* external lines of the linked many-body parts of the symmetrized interaction $\mathcal{K}_V$ will carry renormalization factors $P_m^{1/2}$ or $(1-P_b)^{1/2}$. A remarkably similar result has been obtained independently by Rowe.[89] We should remark, as he does, that similar factors appear on the external lines of the transition amplitude diagrams. [See (7.41) and (D34).]

Second, we should perhaps have distinguished between the "true" and "model" occupation probabilities P_i and $P_i^{(0)}$. We have presumed that the M' summations are defined and carried out within the primary subspace, hence the immediate result involves the model probabilities $P_i^{(0)}$ [see (5.7)] of the primary subspace. But a careful inspection of higher-order diagrams (especially the "many-body vertices" of the primary subspace) reveals terms which convert these into *true* probabilities. This is expected on physical grounds.

Finally, this should be compared with the Green's function result. There one obtains factors of $Z^{1/2}$ instead of $P_m^{1/2}$ or $(1-P_b)^{1/2}$, where $Z=P_m-P_b$ is the *discontinuity* in the distribution P_i at the Fermi surface. One sees from Fig. 2 that $P_m>Z<(1-P_b)$, for states m and b near the Fermi surface, thus we believe that the Green's function theory renormalizes too strongly. The reason, we believe, is that the one-body Green's function is a rather inefficient tool for generating and propagating quasi-particles. It leads to the correct quasi-particle energies, but some amplitude gets lost in the process. This loss is associated with the "background" or "continuum" part of the Green's function, which is often ignored or discarded in Green's function treatments. This awkward feature arises from the necessity of clothing the bare particle to form a quasi-particle (see footnote 79), or in other words from the "unphysical" boundary condition at $t=0$. There is no such difficulty in our time-independent approach, because we deal from the outset with the true eigenstates (or with quasi-stationary states) of the total system. There is no *dynamical* dressing process, and therefore no loss of probability.

Another aspect of the difference between our viewpoint and that of Green's function methodology is illustrated in (8.26).



(8.26)

Term (a) may be regarded as two "irreducible" vertices and a propagator renormalization factor. Term (b) also contains a one-body insertion. The latter is off the the energy shell, however, and its effect is not just a simple numerical factor. In a Green's function treatment this would probably be regarded as a propagator correction, in spite of the fact that it does not factorize completely. Instead, we would regard the entire term (b) as a single "irreducible vertex." But this is partly a matter of semantics.

Summary

We shall summarize the main results of this section.

(1) For open-shell nuclei, this formalism demonstrates that the G-matrix elements are rather insensitive to the number of valence particles. This is an important consideration when the number of valence particles is large.

(2) For nuclear spectroscopy it is important that the lowest unfilled orbitals should exhibit a shell structure of the usual form, instead of behaving like plane waves. This requires the use of a double-partitioning procedure, to distinguish between the "low" configurations of the model subspace, the "medium" configurations which renormalize the model interaction, and the "high" configurations associated with the singular part of the basic interaction v.

(3) For a reasonable partitioning of the full configuration space, any singularities in the formalism can be removed by summing certain sequences of higher-order diagrams. These are diagrams which might otherwise be neglected, so this procedure appears as a natural and useful way of improving the convergence of the series.

(4) These methods allow for a nonsingular and reasonably straightforward treatment of superfluid effects in nuclear matter.

(5) The formalism can be adopted to handle time-dependent situations such as nuclear reactions and the optical potential problem. This fits in very well with the "shell-model continuum" approach to nuclear reactions.

(6) Although originally developed for the problem of open shells, this formalism is useful also for closed-shell systems. Thus for the closed-shell ground state it suggests new ways of selectively summing the Goldstone series to improve the practical convergence of binding energy calculations. This should help to unify the diversity of recent proposals for the binding-energy

[89] D. Rowe, Rev. Mod. Phys. (to be published).

problem, in a way that preserves the best features of the different schemes.

(7) Excitations of closed-shell systems can also be treated, as demonstrated in our discussion of the RPA method.

(8) This formalism provides a fairly complete justification for the Landau theory of Fermi liquids. It provides relations very similar to those established by Green's function methods, the main differences being: (a) cutoffs in the intermediate state integrations are now well-defined. These cutoffs are not associated with the finite lifetimes of "real" quasi-particles because, for a sensible partitioning scheme, the intermediate states are all "virtual". (b) The propagator renormalization effects differ in detail.

The similarities are not at all surprising, because the phenomenological Fermi-liquid theory is essentially just a shell-model description of large systems. The phenomenological theory is based on a set of independent-particle energies ϵ_k, and an effective two-body interaction $f_{kk'}$. The definition $\epsilon_k \equiv (\delta E_{\text{total}})/\delta n_k$ is in complete agreement with the way shell-model workers obtain the "real" particle energies (via stripping and pickup reactions) to be used in spectroscopy calculations. Thus the symbol δn_k corresponds to the *physical addition* or *physical removal* of a particle. The Bloch–Horowitz formalism is very well suited for describing such physical processes. Green's function methods, on the other hand, are based on the *unphysical* processes of adding or removing "bare" particles. This leads to some awkward and unrealistic features.

The most remarkable coincidence, in our opinion, is that the physically interesting phenomena (single-particle excitations, particle–hole correlations, deformations of the Fermi surface, and superfluid correlations) are so similar in all "Fermi-liquid" systems. As a consequence, any formalism which is well adopted for a "first-principles" treatment of nuclei should also apply, at least formally, to liquid He^3. The essential question is whether these methods can converge rapidly enough to be of practical use.

IX. PHYSICAL INTERPRETATIONS, DISCUSSION

Cellular Model

The present derivation also provides a rather straightforward interpretation for these linked-cluster results. This is closely related to the argument, familiar in statistical mechanics, that a large system can be subdivided into many comparatively small subsystems which are still large enough, individually, to be considered approximately independent of each other. This analogy was pointed out by Hugenholtz.[29] To make the discussion more rigorous, we begin by considering a fictitious "cellular" system, where the subsystems are separated from each other by physical barriers. This guarantees *complete independence* for the various subsystems, or "cells," thus the interaction energy is obviously the sum of the subsystem interaction energies,

$$\Delta E = \sum_s \Delta E_s, \tag{9.1}$$

and the wave function is the product of the subsystem wave functions,

$$\Psi = \prod_s \Psi_s. \tag{9.2}$$

In this simple model, the motivations for the various formal manipulations become quite obvious.

To the extent that a large physical system is described by such a model, one immediately concludes that $E \propto N$, and that

$$|\langle \Phi_0 | \Psi \rangle|^2 = \prod_s |\langle \Phi_{0s} | \Psi_s \rangle|^2 \approx e^{-aN}, \tag{9.3}$$

i.e., the probability of finding the system in its "model state" Φ_0 is exponentially small. Alternatively, if Ψ is normalized such that $\langle \Phi_0 | \Psi \rangle = 1$, then $\langle \Psi | \Psi \rangle \approx e^{+aN}$. This is the argument of Hugenholtz.[29] Bethe[47] had previously obtained this result by a more detailed physical argument.

For a cellular system, this enormous wave function renormalization (the fact that Ψ and Φ_0 are almost orthogonal) is obviously nothing to be concerned about. The energy, and also all other expectation values, can be calculated "cell by cell", treating each subsystem separately. Even if one insists on treating the composite system as a single quantum entity, the "other" cells will merely contribute normalization factors which cancel identically in the evaluation of $\langle \Psi | \mathcal{O} | \Psi \rangle / \langle \Psi | \Psi \rangle$, leading one right back to the picture of many separate systems. This aspect of many-body systems has been emphasized by Brueckner.[26] Certainly we should not be surprised at the existence of linked-cluster expansions for Ψ and $\langle \mathcal{O} \rangle$. Convergence need not be a problem either, even for a very large system, since it is only necessary that the perturbation method converges for each of the separate cells. (We may suppose that the overlap $\langle \Phi_{0s} | \Psi_s \rangle$ is fairly large for an individual cell.)

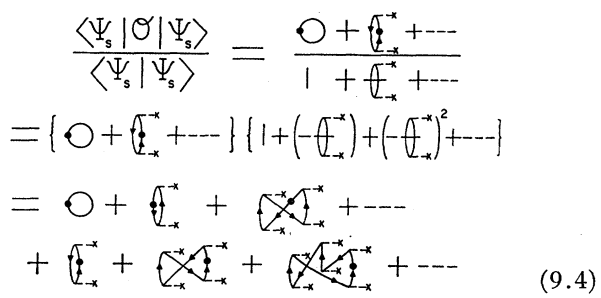
But there must be other ingredients in the interpretation of Goldstone's energy expansion, since this does not take direct advantage of (9.2). This expansion is based on the *unsymmetrical* expression $E = \langle \Phi_0 | H | \Psi \rangle / \langle \Phi_0 | \Psi \rangle$, where the normalization problem is avoided (in the present derivation, although not in Goldstone's) by setting $\langle \Phi_0 | \Psi \rangle = 1$. Starting from the Brillouin–Wigner expansion, as we have done, one feels that it must be possible to eliminate the large energy shifts $\Delta E \propto N$ appearing within the energy denominators. This is because the total energy is also given by the sum of the BW expansions for the separate

subsystems, and in these the denominators include only the small terms ΔE_s. This suggests that we try to relate these "macroscopic" and "microscopic" treatments by expanding the large ΔE's out of the macrosystem denominators. This purely formal step looks suspicious, but it is actually quite justifiable here. The "microscopic" treatment is the physical one, whereas the macroscopic approach, treating noninteracting subsystems as if they were interacting, is obviously artificial. (We assume that the small absolute radius of convergence for a realistic many-body system is connected with the possibility of phase transitions.[59,60] The latter are very strongly inhibited by the physical barriers between the cells of our model.)

Now consider a typical macro-diagram, whose topmost interaction (which represents the V in $\langle\Phi_0|V|\Psi\rangle$) refers to subsystem s. Since the macro and micro expansions must be formally equivalent, it is now clear that all unlinked parts of this diagram coming from sybsystems $s'\neq s$ arose from the need to compensate for the spurious terms $\Delta E_{s'}$ in the denominators of the original expansion. Since these $\Delta E_{s'}$'s now appear within the $(-\Delta E)$ insertions, instead of in the denominators, they clearly must cancel against these unlinked diagrams. The argument of Sec. IV makes this explicit.

The story is not yet complete, however. In removing ΔE from the denominators, we have also removed that small part ΔE_s which belongs to the particular subsystem s labelled by the diagram's topmost interaction. The expansion and cancellation procedure therefore produces some "left-over" diagrams with $(-\Delta E_s)$ insertions. An argument in Sec. III [see especially (3.7) and (3.8)] indicates that these terms must correspond to certain of the exclusion-violating (e.v.) terms in the Goldstone expansion for this cellular system. Here we must distinguish between *essential* and *inessential* e.v. terms. Consider the exchange diagram obtained by crossing (or uncrossing) a pair of lines with the same label. If the resulting diagram is also linked, then both of these e.v. terms are inessential. Since these exchange terms cancel identically, they could just as well have been omitted in the first place. Their only purpose is to simplify the diagram rules, permitting independent summations over all the single-particle labels. On the other hand, if the resulting exchange diagram is unlinked (and therefore not in the Goldstone expansion), the original e.v. diagram is essential. The left-over RS diagrams mentioned above, linked but with $(-\Delta E_s)$ insertions, correspond to the essential e.v. diagrams where exclusion is violated by two or more *holes* in the same normally occupied state m. (The essential e.v. terms involving particle states b are discussed at the end of this subsection.)

Now consider the Thouless expansion (6.9) for a general expectation value, $\langle\mathcal{O}\rangle$, for the same cellular system. There are now two types of essential e.v. terms to consider. First, there are those where the "unlinked parts," which would be obtained by uncrossing the identical lines, do not overlap the level of the $\mathcal{O}$ interaction. These are similar to those already discussed—the terms with crossed *hole* lines represent the removal of ΔE_s from the energy denominators. (Crossed particle lines are discussed below.) Secondly, there are essential e.v. terms where the "unlinked parts" overlap the level of the $\mathcal{O}$ operator. Such terms, with crossed *hole* lines, represent a perturbation expansion of the normalization denominator in $\langle\Psi_s|\mathcal{O}|\Psi_s\rangle/\langle\Psi_s|\Psi_s\rangle$. This is illustrated in (9.4), for the case of a "cell" containing only one particle.



(9.4)

Here the dots represent a one-body operator, kinetic energy for example. Horizontal lines are used in the normalization diagrams to indicate the level where the wave function parts $\mathbf{W}$ and $\mathbf{W}^\dagger$ are joined. This type of expansion was used explicitly in Sec. VII.

We shall now try to complete the relation of this cellular model to actual many-body systems. One obviously cannot identify the "independent subsystems" with definite regions of space, when the physical barriers of the model are not actually present, since the single-particle orbitals now extend over the entire volume. Nevertheless, each linked-cluster term behaves very much like an independent subsystem. The essential point is that the interactions between different clusters are *strictly negligible*, by definition. Such events are described by other terms in the expansion, namely the linked clusters which involve all the particles of the original two clusters. The clusters can interact in two ways. First, there are the *dynamical* interactions, those involving the perturbation V. But the clusters can also interact *statistically*, since they must all share the same set of intermediate states b. This is our interpretation for the essential e.v. terms with crossed *particle* lines.

Partial Summations

This cellular model can also be helpful in visualizing the meaning of various partial summations. The above picture of a many-body system should be reasonably correct for a weak enough perturbation V. In almost all

practical applications, however, (with the possible exception of atomic structure[90]) the expansion in powers of V will not converge, and one must resort to partial summations and analytic continuation arguments.[59,60] Another important reason for these summations is that they provide closed mathematical expressions for prominent physical features of the system. In terms of the preceding discussion, each partial summation amounts to grouping an infinite number of linked cluster terms together into a single "cell," which is then treated by nonperturbative methods. The role of the original expansion in V, then, is simply to provide a framework for splitting the system up into smaller units which can be treated mathematically as independent subsystems.[11] In other words, the original expansion is to be regarded simply as a bookkeeping device. One usually thinks of doing these summations when V is weak or otherwise well-behaved, and then analytically continuing the result for each separate "cell". The best known of these summations are: (a) "upgoing ladders" of two-body v interactions,[26,28] forming the reaction matrices which various authors denote by t, K, or G; (b) self-energy insertions, leading to effective single-particle potentials[26,28]; and (c) the ring diagrams of the so-called random phase approximation.[91,92,41,42] Less familiar, but also useful in the nuclear many-body problem are: (d) "generalized time ordering" (Sec. IV and Refs. 9, 48), putting certain parts of a diagram on the energy shell; (e) Bethe's summation of three-body cluster terms[11]; (f) summations describing wave function renormalization [see (9.4)] and true single-particle occupation probabilities (subsection below); and (g) enlargement of the quasi-degenerate subspace D.

In enlarging D, for example by converting some of the lowest intermediate states (or highest normally occupied states) into valence states, one is, in effect, grouping together all cluster terms whose smallest energy denominators are less than some specified minimum. This "cell" is then treated by solving the valence or shell model secular equation (5.13). (This cell itself can often be subdivided by the methods of Sec. VII.) Although it may be stretching a point to consider this a "partial summation", it is interesting to see what types of summations this corresponds to. Consider a grossly oversimplified problem, a non-degenerate one-body system with only two unperturbed states, Φ_0 and Φ_1. All terms beyond second order in the Brillouin–Wigner expansion will consist of a number of self-energy insertions, V_{11}, in the upgoing line of the second-order diagram. The whole series is therefore

$$E=E_0+V_{00}+V_{01}\frac{1}{E-E_1}\sum_{n=0}^{\infty}\left(V_{11}\frac{1}{E-E_1}\right)^n V_{10}, \quad (9.5)$$

or

$$E-(E_0+V_{00})=V_{01}[E-(E_1+V_{11})]^{-1}V_{10}, \quad (9.6)$$

which is clearly just the condition for the vanishing of the 2×2 secular determinant. Now consider a similar system with three unperturbed states, Φ_0, Φ_1, and Φ_2. The first step is to sum out the first-order insertions V_{11} and V_{22}, as before. The intermediate states of the remaining diagrams must then alternate between Φ_1 and Φ_2. Repeated alternations, 121212 etc., can be eliminated by summing out the second-order insertions $V_{12}V_{21}$ and $V_{21}V_{12}$, the final result being

$$\begin{aligned}E=&E_0+V_{00}\\&+\{V_{01}+V_{02}[E-(E_2+V_{22})]^{-1}V_{21}\}(E-\mathcal{E}_1)^{-1}V_{10}\\&+\{V_{02}+V_{01}[E-(E_1+V_{11})]^{-1}V_{12}\}(E-\mathcal{E}_2)^{-1}V_{20},\end{aligned} \quad (9.7)$$

$$\mathcal{E}_1\equiv E_1+V_{11}+V_{12}[E-(E_2+V_{22})]^{-1}V_{21}, \quad (9.8)$$

which is equivalent to the 3×3 secular equation. A systematic extension of this argument would lead to the Feenberg–Feshbach[93,94] form of perturbation theory, but of course we are more interested in expressing the result in the equivalent secular matrix form.[95]

After employing the above techniques to organize the system into a convenient set of "cells," it would seem advantageous to replace the Goldstone energy denominators by the BW-type denominators appropriate for each cell, in effect reversing the arguments of Sec. III. This would surely improve the practical rate of convergence. It is usually not feasible to carry this out completely, but a wise choice of single-particle potentials for the normally occupied states generally represents an important step in this direction. The familiar hole-bubble insertions of nuclear matter theory[48,9] and the diagonal hole–hole ladder which Kelly[90] has summed both have precisely this character. It was shown in Sec. VIII that partial summations of this type (now representing the cell's contribution to ΔE_V) are useful for eliminating the problem of vanishing energy denominators in the expansion of $\mathcal{U}_V$.

[90] H. P. Kelly, Phys. Rev. **136**, B896 (1964); H. P. Kelly, in *Advances in Theoretical Physics*, K. A. Brueckner, Ed. (Academic Press Inc., New York, 1966), Vol. 2.

[91] M. Gell-Mann and K. A. Brueckner, Phys. Rev. **106**, 364 (1957).

[92] T. D. Schultz, *Quantum Field Theory and the Many-Body Problem* (Gordon and Breach Science Publishers, New York, 1964).

[93] E. Feenberg, Phys. Rev. **74**, 206 (1948); R. I. Richards, *ibid.* **74**, 835 (L) (1948); H. Feshbach, *ibid.* **74**, 1548 (L) (1948); E. Feenberg (unpublished lecture notes).

[94] P. M. Morse and H. Feshbach, *Methods of Theoretical Physics* (McGraw-Hill Book Co., Inc., New York, 1953), Vol. II, p. 1010.

[95] For an infinite-dimensional subspace D, this procedure would require an infinite number of partial summations. This is probably the reason why no one has yet succeeded in obtaining the BCS theory by partially summing Goldstone diagrams. Nevertheless, something rather similar to the BCS theory has been obtained by summing the diagrams of statistical mechanics: A. Katz, Nucl. Phys. **42**, 394 and 416 (1963).

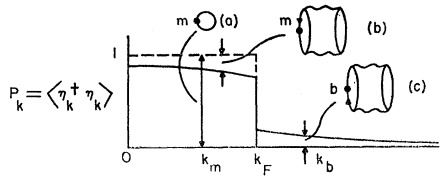


FIG. 2. Momentum distribution of a normal system. The leading diagrams in the Thouless expansions for P_m and P_b are shown.

Small Systems

It seems appropriate, at this point, to inquire how large a system must be before linked-cluster methods become preferable to a Brillouin–Wigner expansion (unlinked), for example, or even a direct variational calculation. The BW expansion is clearly the best (most rapidly converging) for the one-body problem of Sec. III. The cellular model answers this question quite directly. Linked-cluster methods should be preferable whenever the system is divisible into cells or clusters (by "cluster" we mean here one or more diagrams with a particular set of normally occupied states), such that (a) more than one cell makes a significant contribution to the interaction energy and (b) the largest number of particles for any clusters which contribute significantly must be less than the total number of particles. If (b) is not satisfied it might be better to calculate the entire system directly, by means of a variational wave function for example.

For the nuclear problem it appears at present that three-body clusters must be calculated rather carefully,[11] even though their net effect is probably small, but that four-body clusters should be quite negligible. (We are referring to the very-short-range correlations induced by the repulsive core. These have little or nothing to do with the special problem of alpha-particle clustering in the nuclear surface.[96] There is evidence[97] that the latter can be treated by conventional shell-model methods, presumably by some extension of the usual treatment of nuclear pairing.) Thus it appears that nuclear matter methods should be appropriate even for He^4. These methods have been applied to He^4 by Mang, Wild, and Beck[6], and by Wong.[12] In such a light nucleus it is very important to take account of the spurious center-of-mass motion.[6]

Even if the four-body cluster term in He^4 should turn out to be not quite negligible, it is surely so small that a comparatively crude calculation should suffice. The virtue of the linked-cluster approach is that it distinguishes clearly between "large" and "small" contributions.

[96] G. Igo, L. F. Hansen, and T. J. Gooding, Phys. Rev. **131**, 337 (1963); H. Dubost, M. Lefort, P. Peter, and X. Tarrago, Phys. Rev. **136**, B1618 (1964).

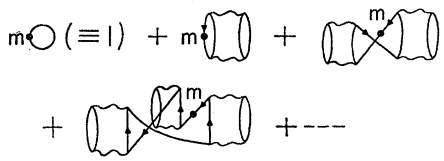
[97] K. Harada, Progr. Theoret. Phys. (Kyoto) **26**, 667 (1961); and **27**, 430 (1962).

Single-Particle Occupation Probabilities

One of the most important features of a many-body system is its distribution of single-particle occupation probabilities, or true occupation numbers, $P_i = \langle \eta_i^\dagger \eta_i \rangle$.[98] For an infinite system this is commonly called the momentum distribution. Consider the ground state of normal nuclear matter. (We shall assume, for the moment, that nuclear matter is normal.) Nondegenerate methods are appropriate here, so the distribution is given by Thouless's linked expansions for the number operators $\eta_k^\dagger \eta_k$. The leading diagrams of these expansions are shown in Fig. 2; their interpretation should be quite clear.

Note that diagrams (b) and (c) are the same except for the location of their number operators. One finds therefore, after summing over all indices, that their contributions to $\sum_m P_m$ and to $\sum_b P_b$ are equal and opposite. [Note the sign difference due to the extra hole line segment in (b).] This same phenomenon occurs in all diagrams.[99] Consider a particular intermediate level of a particular Goldstone energy diagram. If one inserts number operators successively into each of the single-particle lines at this level, the sum of all these terms will always be zero. The total number of particles, $N = \sum_i P_i$ is therefore conserved, separately, by each of these sets of diagrams.

For normal nuclear matter, the diagrams in Fig. 2 should provide a fairly good approximation to the true momentum distribution. But there are many other terms to consider, even if we restrict the discussion to two-body correlation effects. There is a whole geometric series of two-body correlation terms, quite analogous to the situation in (9.4). For $k_m < k_F$, we find



$$= [1 + \Omega^{-1} \textstyle\sum_n \langle \zeta_{mn} \mid \zeta_{mn} - \zeta_{nm} \rangle]^{-1}. \qquad (9.9)$$

But there are also terms of the form

(9.10)

[98] This quantity is usually denoted by n_i, although some authors use this symbol for the *model* (or quasi-particle) occupation numbers (5.7). We have already used n in several different ways, hence the symbols P_i for *true* and $P_i^{(0)}$ for *model* occupation probabilities may reduce confusion.

[99] A. Klein, *Lectures on the Many-Body Problem* (Naples, 1962), E. R. Caianiello, Ed. (Academic Press Inc., New York, 1962).

whose net effect is to replace (9.9) by

$$P_m=[1+\Omega^{-1}\sum_n\langle\zeta_{mn}\mid\zeta_{mn}-\zeta_{nm}\rangle P_n]^{-1}. \quad (9.11)$$

For an orientation, we shall average over all indices and replace[100]

$$\Omega^{-1}\sum_n\langle\zeta_{mn}\mid\zeta_{mn}-\zeta_{nm}\rangle$$

by

$$\kappa\equiv\rho\langle\zeta_{mn}\mid\zeta_{mn}-\zeta_{nm}\rangle_{\text{Av}}. \quad (9.12)$$

Then

$$\bar{P}^{-2}-\bar{P}^{-1}-\kappa=0, \quad (9.13)$$

$$\bar{P}^{-1}=\tfrac{1}{2}[1+(1+4\kappa)^{1/2}], \quad (9.14)$$

and

$$\bar{P}=1-\kappa+2\kappa^2-5\kappa^3+\cdots. \quad (9.15)$$

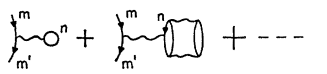
In nuclear matter,[101] $\kappa\approx 0.15-0.18$. One can iterate (9.11), replacing P_n by $\bar{P}$ etc., to get some idea of how P_m depends on m. By the same token, diagram (c) of Fig. 2 should be multiplied by P_mP_n before summing over the hole lines. This discussion can obviously be extended to include the effects of 3, 4, $\cdots$, n-body correlations.

A careful treatment of P_m, along the lines indicated here, is necessary for an accurate determination of the shell-model potential.[9] This should also be quite important in any applications of the theory to liquid He^3, since the parameter κ is surely much larger there than in nuclear systems.[102]

Generalized Time Ordering

To carry out the summations in (9.9) and (9.11), we have had to use the generalized time ordering (g.t.o.) treatment discussed in Sec. IV. In other words we have used the factorization theorem, summing together all possible relative time orderings of the v-interaction ladders belonging to the different two-body correlation parts in $\mathbf{W}(\mathbf{W}^\dagger)$, denoted by $|\zeta\rangle(\langle\zeta|)$, which lie entirely below (above) the level of the number operators $\eta_m^\dagger\eta_m$. This should be obvious from the analogy with (9.4).

The true occupation probabilities P_m play an important role in the theory of finite nuclei.[9] The shell-model potential which a normally occupied state m feels is due mainly to the lowest-order insertion. This is formally the same as the Hartree–Fock potential, except that the "bare" interaction v is replaced by an effective two-body interaction, the Brueckner reaction matrix. We see now that the effect of many of the higher-order insertions is simply to renormalize this so-called Hartree–Fock term[2–4] in V_{SM}. This takes account of the finite probability that state n is unoccupied due to correlations within the sea of "background" particles.[43] Thus



$$\rightarrow\sum_n\langle m'n\mid G\mid mn-nm\rangle P_n\approx\langle m'\mid V_{\text{HF}}\mid m\rangle\bar{P}. \quad (9.16)$$

The correction $(\bar{P}-1)V_{\text{HF}}$ is closely related[43,8] to the "rearrangement potential" introduced by Brueckner and Goldman.[3]

The reaction matrix in the V_{HF} term can also be put entirely on the energy shell by the g.t.o. treatment. It should be clear now that the g.t.o. treatment of selected classes of Goldstone diagrams has the following benefits: (i) The partially summed series is more rapidly convergent. (ii) The g.t.o. diagrams are easier to evaluate, thanks to the elimination of some (and sometimes all) of the off-energy-shell effects. (iii) This treatment often leads to expressions with a simple physical interpretation, as in (9.11) and (9.16). But some caution is necessary. In each g.t.o. application it is important to check that there is still a one-to-one correspondence between the terms of the old and new expansions. The problems of "double counting" are discussed in Refs. 9 and 48.

Insertions similar to (9.16) also exist for the valence particles (or valence holes) of open-shell nuclei, and again they will make the largest contribution to the V_{SM} acting on these particles. But here we observe that the factorization theorem does not apply to valence diagrams of the original Bloch–Horowitz expansion, due to the unfortunate presence of ΔE_V in all the valence denominators. The "reduced" BH expansion (Sec. V), however, does allow a g.t.o. treatment of all diagrams of the type (9.9) to (9.11) which appear in (9.16). Thus the reduced BH expansion allows for the simple P_n renormalization of the V_{HF} insertion. This is important from the standpoint of physical interpretation. The reaction matrix in V_{HF} is still off the energy shell by the amount ΔE_V, however, and this may be troublesome if there are many valence particles. This difficulty is avoided by the expansion in Sec. VII. Note that the diagrams discussed here are all examples of the topological structures shown in (a) and (b) of (4.8).

Existence of Fermi Surface, Phase Transitions

The most striking feature of Fig. 2 is that the Fermi surface still exists. (This is by assumption, of course, since this is the definition of a normal system.) The discontinuity at k_F persists in spite of the strong interactions. In terms of the expansion $\Psi=\sum_i a_i\Phi_i$ of Sec. II, where the Φ_i's are N-body Slater determinants,

[100] For discussions of the two-body distortion wave function ζ, see Refs. 48 and 101.

[101] G. Dahll, E. Østgaard, and B. Brandow, Nucl. Phys. (to be published).

[102] Recent calculations by E. Østgaard (private communication) indicate that $\kappa\approx 0.25$ for liquid He^3. Thanks to statistical weighting factors, this is not as large as one might have feared. This is quite encouraging for future calculations of liquid He^3.

this indicates that the unperturbed state Φ_0 is still the dominant one. Of course its amplitude is extremely small, $|a_0|^2 \approx e^{-aN}$, where $a \approx \frac{1}{2}\kappa$ [to lowest order in κ, see (9.12)], but this state dominates in the sense that the *ratios* $|a_i/a_0|^2$ are also extremely small for all $i \neq 0$. This is easily seen for nuclear matter, where a typical Φ_i has around 15% of the particles excited out of the Fermi sea. It is easily seen that the number of ways of choosing $\frac{1}{2}\times 0.15N$ pairs of particles out of N particles increases far more rapidly (factorially so) than $\exp(\frac{1}{2}\times 0.15N)$. Let the former number be $\mathfrak{N}$. Then

$$|a_0|^{-2}\sum_i |a_i|^2 \approx \mathfrak{N}\,|a_i/a_0|_{\text{AV}}^2 \approx \exp(\tfrac{1}{2}\times 0.15N) \quad (9.17)$$

implies that $|a_i/a_0|_{\text{AV}}^2$ is extremely small. Consideration of the large number of intermediate orbitals a, b which each pair m, n can scatter into can only strengthen this conclusion.

This argument assumes that there is no coherence between *different* correlated pairs. Any coherence between excited pairs would be described by four, six, eight-body clusters, etc., which should be negligible. [The coherence included within the P_m of (9.11) is only of the most trivial sort, namely that a particle can interact pairwise with only one other particle at any instant.] But there *is* a coherence between the parts of the various Φ_i's referring to the majority (roughly 85%) of the particles remaining unexcited. This coherence is responsible for the discontinuity at k_F.

It may seem strange, at first, that an exponentially small part of Ψ can still have a dominating influence. But for normal nuclear matter, where only the two-body correlations are strong, the explanation is really obvious. This small part, Φ_0, contains all the long-range order.

It is interesting to compare this situation with other many-Fermion systems, for example the high-density electron gas. Here the momentum distribution[65] is very similar to that in Fig. 2, except that the important correlations now come from the "ring" diagrams. The higher-order ring diagrams involve arbitrarily large numbers of particles, thus the possibility arises that these correlations could extend out to very long range. Indeed, the formulation of Sawada[103] and Wentzel[104] shows that these diagrams are closely related to the collective vibration modes (plasmons), where this long-range correlation is actually realized. In the ground state, however, these diagrams simply represent a screening of the long-range part of the Coulomb interaction.[41,42,92] Each electron is surrounded by a polarization charge whose density varies roughly as $e^{-\mu r}/r$, where μ^{-1} is comparable to the interparticle spacing.[105] Each electron is, to some degree, avoiding all its neighbors, and this clearly requires the cooperation of *all* the electrons. This is why high-order rings occur even though the phenomenon is short range. The success of the perturbation-partial-summation treatment of Gell-Mann and Brueckner[91] would again seem to be the result of having a long-range order which is completely described by Φ_0.

The situation is very different for systems with a BCS ground state. Any perturbation-partial-summation treatment is bound to fail, if the starting point is Φ_0, because of the strong admixture of many low-lying Φ_i's. But linked-cluster methods can still be used (Sec. VIII) if one first separates these low Φ_i's off into a quasi-degenerate subspace. The lesson seems to be that one must choose this subspace D to include all the long-range order within the projection or "model" wave function, $\Psi_D = P\Psi$.

It is also instructive to consider the differences between these last two examples, high-density electron gas and superfluid system, in terms of the secular matrix. The reason why Φ_0 provides a suitable starting point in only the former of these examples is demonstrated by a simple schematic model where the effective interaction matrix $\mathcal{V}$ is finite-dimensional, with all of its elements equal to a constant v_0. It is well known[106] that this model has one "collective eigenstate" consisting of a strong admixture of all the unperturbed Φ_i's. The other eigenstates are each dominated by some particular Φ_i, with comparatively weak admixtures of the other unperturbed states. (In this simple model, the "purity" of the noncollective states increases with the dimension of the secular matrix.) The high-density electron gas corresponds to $v_0 > 0$. The collective modes (plasmons) therefore occur at high energy, while the ground state remains dominated by Φ_0. Thus it is not too surprising that the ground-state correlations are weak enough to be handled as perturbations. A superfluid system corresponds to $v_0 < 0$, so the ground state is now the "collective" one. This is conspicuously lower in energy than any other state (the BCS gap), and it contains many low-lying Φ_i's with amplitudes comparable to Φ_0, invalidating perturbation treatments based on the latter.

These qualitative arguments strongly support the idea that the breakdown of perturbation-partial-summation methods is ultimately due to phase changes, i.e., changes in the long-range order. This is consistent with the uncertainty principle: Short-range order involves high momentum components and therefore high energies, while the components that determine long-range order are nearly degenerate. Thus one expects that phase changes are signalled by unavoidable divergences somewhere in the formalism. The connection between a divergence of the Brueckner reaction matrix and a BCS ground state, for example, has often

[103] K. Sawada, Phys. Rev. **106**, 372 (1957).
[104] G. Wentzel, Phys. Rev. **108**, 1593 (1957).
[105] For corrections to this simple picture, see J. S. Langer and S. H. Vosko, J. Phys. Chem. Solids **12**, 196 (1959); W. Kohn and S. H. Vosko, Phys. Rev. **119**, 912 (1960).
[106] B. R. Mottelson, *The Many-Body Problem* (Les Houches, 1958), C. DeWitt, Ed. (Dunod Cie., Paris, 1958); J. R. Schrieffer, *Theory of Superconductivity* (W. A. Benjamin, Inc., New York, 1964); G. E. Brown, Ref. 18.

been discussed.[107] Thouless[108] has extended this discussion to finite temperatures; in fact he was able to obtain the BCS critical temperature expression from this criterion.

Other well-known studies of this sort are those of Luttinger and Nozieres.[109] Following an observation by Migdal,[110] they have shown in detail that the existence of the Fermi surface, and all that this implies in terms of low-temperature properties, follows from the assumption that perturbation theory makes sense, i.e., that certain partial summations[111] lead to reasonable results. Prior to these studies, the existence of the Fermi surface in metals had been considered a paradox, just as the success of the nuclear shell model has seemed so paradoxical.

We propose (a) that the conditions of Thouless, Migdal, and Luttinger are equivalent to the condition (2.15) for $\Psi_D=\Phi_0$, and (b) that (2.15) is the natural generalization of this argument. It is very doubtful whether these claims can ever be established with mathematical rigor, but we would like to add one more plausibility argument. In mathematics, the possibility of continuing a function analytically depends on the possibility of choosing a sequence of points, where each point lies within the radius of convergence of the power series expansion around the previous point. The perturbation-theoretic equivalent is to break up the total perturbation into a sum of much weaker ones

$$V=\sum_{p=1}^{P} V_p, \tag{9.18}$$

such that convergent expansions exist for all members of the sequence

$$\Psi(\sum_{p=1}^{P'} V_p)\rightarrow\Psi(\sum_{p=1}^{P'+1} V_p). \tag{9.19}$$

The radius of convergence of an ordinary perturbation expansion is usually determined by the nearest point where a level crossing or accidental degeneracy occurs.[94] One therefore expects that such a sequence can always be found, unless the system undergoes a sudden phase change of some sort as the total perturbation reaches a certain critical strength. (We are thinking here in terms of finite systems. Of course this critical strength may approach zero very rapidly with increasing size of the system, as in the famous BCS example.) We argue that such a phase change corresponds mathematically to the breakdown of condition (2.15) for some particular D. Finally, it seems quite plausible that if such a convergent sequence (9.19) exists, for some choice of H_0 and D, that it may then be possible, for practical purposes, to replace this by a sequence of partial summations. The latter are simply a more convenient way of doing the analytic continuation. For further discussion along these lines, we refer to the papers of Katz[60] and Baker.[59]

"Model" and "True" Descriptions

We have seen that Goldstone's energy expansion is based on the *unsymmetrical* expression

$$E=\langle\Phi_0\,|\,H_0+V\,|\,\Psi\rangle/\langle\Phi_0\,|\,\Psi\rangle, \tag{9.20}$$

where Ψ is the true wave function and Φ_0 is an eigenstate of H_0. This has the great advantage of expressing the total energy in terms of a *model* energy

$$E_0=\langle\Phi_0\,|\,H_0\,|\,\Phi_0\rangle\equiv\langle H_0\rangle_m, \tag{9.21}$$

and the expectation value of a *model* interaction $\mathcal{U}=V\Omega$ taken with respect to the *model* wave function,

$$\Delta E=\langle\Phi_0\,|\,\mathcal{U}\,|\,\Phi_0\rangle\equiv\langle V\rangle_m. \tag{9.22}$$

The various Bloch–Horowitz expansions extend this model description to degenerate systems. On the other hand, the total energy is also expressible in terms of the *true* expectation values, $\langle H_0\rangle_t$ and $\langle V\rangle_t$, which follow from the *symmetrical* expression

$$E=\langle\Psi\,|\,H_0+V\,|\,\Psi\rangle/\langle\Psi\,|\,\Psi\rangle. \tag{9.23}$$

Linked expansions are available (Secs. VI and VII) for calculating $\langle H_0\rangle_t$ and $\langle V\rangle_t$.

These "model" and "true" descriptions are related by a simple mathematical transformation. One finds, either from the argument (6.10), (6.11), or by direct differentiation of (9.23), that[66]

$$dE_\lambda/d\lambda=\langle\Psi_\lambda\,|\,V\,|\,\Psi_\lambda\rangle=\langle\lambda V\rangle_t/\lambda, \tag{9.24}$$

where $H_\lambda=H_0+\lambda V$, assuming $\langle\Psi_\lambda\,|\,\Psi_\lambda\rangle=1$ for all λ. Integration then leads to[112]

$$\langle V\rangle_m=E_{\lambda=1}-E_{\lambda=0}=\int_0^1\frac{\langle\lambda V\rangle_t}{\lambda}\,d\lambda. \tag{9.25}$$

What this means is that the nth order perturbation terms in $\langle V\rangle_t$ are exactly the same as those in $\langle V\rangle_m$, but multiplied by a factor of n. This is easily understood diagrammatically. The Wick algebra leads to diagrams of exactly the same topogloical form for both $\langle V\rangle_t$ and $\langle V\rangle_m$. But the former V^n diagrams occur n times more often, because the V which appears explicitly in $\langle V\rangle_t$

[107] C. T. DeDominicis, Ph.D. thesis, University of Birmingham, 1957 (unpublished); J. Goldstone, Ph.D. thesis, Cambridge, 1958 (unpublished); L. Van Hove, Physica **25**, 849 (1959). The latter contains an extensive list of references. See also Refs. 42, 60, and 81.

[108] D. J. Thouless, Ann. Phys. (N.Y.) **10**, 553 (1960).

[109] J. M. Luttinger, Phys. Rev. **119**, 1153 (1960); and **121**, 942 (1961); P. Nozieres and J. M. Luttinger, Ref. 73.

[110] A. B. Migdal, Zh. Eksperim. i Teor. Fiz. **32**, 399 (1957) [English transl.: Soviet Phys.—JETP **5**, 333 (1957)].

[111] These partial summations are the ones which give the self-energy operator $\Sigma(k,\omega)$. Except for the "causal" boundary conditions brought in by the field-theoretic formalism, this operator is essentially the same as the quantity $F_V(E_{0V}+\Delta E_V)$ of (6.15), calculated for a *single* valence particle by means of the *reduced* BH formalism. The latter is mathematically equivalent to the one-body linked parts of $\mathcal{U}_V$, for systems with an arbitrary number of valence particles. [Note the comment below (8.24).]

[112] This has been attributed to Pauli. See also T. Kinoshita and Y. Nambu, Phys. Rev. **94**, 598 (1954), and K. Sawada, Ref. 103.

can now correspond to *any* of the n interactions in the diagrams. (The V in $\langle V\rangle_m$ always corresponds to the topmost interaction of these diagrams.)

Note that $\langle H_0\rangle_m$ and $\langle V\rangle_m$ are both well-behaved and easy to visualize, which is generally *not* true of $\langle H_0\rangle_t$ and $\langle V\rangle_t$. These "true" quantities are generally considerably larger, and with opposite signs. One must therefore work considerably harder to obtain a specified degree of accuracy for their sum, E, than with the "model" description.

On the other hand, the familiar Raleigh–Ritz variational method requires a *symmetrical* energy expression, as in the "true" description. One should therefore be very cautious about applying variational arguments to approximations based on these linked expansions. At first sight, it appears that variational arguments cannot have any formal validity here. Empirically, however, they lead to a rather successful description of finite nuclei.[3–5,7,12–14] This paradox can be resolved by noting that the Taylor expansion for the *total* energy, in powers of V, is unique. The "true" and "model" expansions must therefore be formally equivalent, when the *entire* expansions are considered. Differences can arise only from the way these series are terminated. We shall show elsewhere that the types of partial summations commonly employed in nuclear matter theory can easily be arranged so that the resulting energy expression possesses stationary properties closely related to the Raleigh–Ritz principle. In fact, it is possible to construct a whole hierarchy of these "stationary approximations", whose limiting form is precisely the Raleigh–Ritz principle. The evidence for this is the mass operator variational principle discussed in Ref. 9. The arguments behind these statements are summarized in the next section.

The distinctions between the true and model descriptions have been emphasized by Prange and Klein.[113] These distinctions are also very important for comparisons with the other formalisms developed for nuclear matter.[114] The Jastrow method[23] and the Green's function method[80] both employ the true description, whereas Mohling's expansion[115] corresponds to the model description.

X. FORMAL DEFINITION OF THE SHELL-MODEL POTENTIAL

A "fundamental" theory of nuclei requires that the theory of nuclear matter be extended in three ways: (i) A degenerate version of the Goldstone expansion is required for open-shell nuclei. This has been fully discussed above. (ii) Numerical methods must be developed to handle the new problems arising from the finite geometry. The progress here is also quite encouraging.[116] (iii) A satisfactory formal definition of the shell-model potential $V_{\rm SM}$ is needed. The general program is to use many-body perturbation theory, starting from a one-body "model" Hamiltonian $H_0=T+V_{\rm SM}$, and a perturbation $V=v-V_{\rm SM}$. One sees that $V_{\rm SM}$ is essentially a "free parameter" in the perturbation formalism.[47] We shall now discuss the problem of finding a suitable choice for this $V_{\rm SM}$.

Closed-Shell Nuclei

One expects the theory of closed-shell nuclei to look rather similar to the familiar Hartree–Fock theory. We shall therefore consider the possibilities for determining $V_{\rm SM}$ by extending the concept of the Hartree–Fock potential. The latter can be obtained in several different ways: (a) The variational approach—minimizing $\langle H\rangle$ with respect to the class of all single-determinant wave functions Φ_0. (b) Choosing Φ_0 such that the first-order perturbation terms in $(\Psi-\Phi_0)$ shall not include any terms where only a single particle is excited out of the initial configuration (Brillouin's theorem).[42] (c) In the linked-cluster language, $V_{\rm HF}$ is chosen to cancel all diagrams containing first-order insertions.[28]

We first consider generalizations of the variational argument (a). The introduction of certain partial summations (and orthogonality requirements) followed by a termination of the Goldstone expansion, can be arranged to give a functional for the total energy, $E_{\rm tot}(\{\phi_m\})$, in which the normally occupied orbitals ϕ_m play the role of variational parameters. One can then minimize this with respect to the ϕ_m's just as in ordinary Hartree–Fock theory. This leads to a very simple and intuitively pleasing explanation for the shell model,[3,4] *provided* that one relies on the local density approximation of Brueckner, Gammel, and Weitzner.[2] But this approach is not at all simple if one tries to work *consistently* within the finite geometry of the shell model.[8] Given an orthonormal set $\{\phi_m\}$, one must set up some self-consistency conditions to complete the definition of H_0, in other words to define the unoccupied orbitals ϕ_b as well as all the single-particle energies E_m, E_b. One must then ensure, either directly or by means of Lagrange multipliers, that the complete basis $\{\phi_m, \phi_b\}$ remains orthonormal *during* the variation of the ϕ_m's.

There are really two basic difficulties here. The first is that variational arguments, by themselves, give no indication of how the self-consistency conditions should be chosen to complete the definition of H_0. The second difficulty is that the energy expansion must be terminated in a way consistent with the "true" form of energy expression (9.23), as required by the Raleigh–Ritz principle. Thus the variational approach is incomplete. It is unable, by itself, to provide a sound theory of the shell model. Brueckner and collaborators[2–4] have

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

[114] The other nuclear matter formalisms are evaluated in the review articles of Petschek and of Bell and Squires, Ref. 1, and also in Ref. 9. A number of other formalisms are discussed by Kumar, Ref. 1.

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

[116] See especially Refs. 2, 8, 10, 12, and 24.

managed to avoid these problems by regarding their local density approximation as an *ansatz*. Taken in this sense, the argument of Brueckner and Goldman[3] is perfectly valid.

The other approaches, (b) and (c), are closely related, but we shall now argue that (c) is much more general than (b). Nesbet[117] and Löwdin[118] have pointed out that the Brillouin condition (b) can easily be generalized. They propose that Φ_0 should be defined such that, to *all* orders of perturbation theory, the expansion $\Psi=\sum_i a_i\Phi_i$ contains no determinants with only a single particle excited out of the initial configuration. This amounts to saying that V_{SM} should be defined by the sum of all diagrams (or single-particle insertions) whose net effect is to produce a single particle–hole pair. This is an important and useful idea, but, like the variational approach, it is incomplete. To obtain the actual orbitals ϕ_m, ϕ_b which diagonalize $H_0=T+V_{\mathrm{SM}}$, one also needs the matrix elements $\langle m' \mid V_{\mathrm{SM}} \mid m\rangle$ and $\langle b' \mid V_{\mathrm{SM}} \mid b\rangle$. But these are not determined by the Brillouin condition.

When the original Brillouin argument is examined more carefully,[42] one finds that the Hartree–Fock potential has, in effect, *already* been defined to be just the insertions ("direct" and "exchange") of first order in v. In this sense, the Brillouin condition is not really a statement about V_{HF} at all. It refers instead to the properties of the basis $\{\phi_m, \phi_b\}$ which diagonalizes $H_0=T+V_{\mathrm{HF}}$.

How, then, can this argument be extended to higher orders in v? The most plausible procedure is to argue that, since the generalized Brillouin condition is satisfied when the "particle–hole" matrix elements $\langle b \mid V_{\mathrm{SM}} \mid m\rangle$ are defined by the sum of all the one-particle insertions, the "hole–hole" and "particle–particle" matrix elements should *also* be defined in this way. But this prescription is really quite impractical. The trouble is that the diagram rules often lead to different energy denominators when the insertions occur in different "corners" (m', m), (b, m), and (b', b) of the V_{SM} matrix. Some of these insertions can be put entirely on the energy shell by the g.t.o. factorization, but many of them cannot. An off-energy-shell insertion is strongly dependent on the "local excitation energy" within the skeleton at the level where it is inserted. This means that it cannot be interpreted as a potential in the usual sense.

The diagram cancellation argument, (c) above, includes (b) as a special case. It places *all* the matrix elements of V_{SM} on an equal footing, instead of focussing special attention on the "particle–hole" elements. This permits considerable flexibility because, according to this view, V_{SM} is not subject to any *a priori* requirements beyond that of Hermiticity. It is a "free parameter," which can be chosen to optimize the convergence of the expansion.[47] The "optimum" choice might then depend somewhat on which terms in the expansion one is able (or willing) to calculate explicitly. This flexibility can be used, for example, to include some important three-body cluster effects in an approximate manner,[11] along the lines first proposed by Rajaraman.[88] It is interesting that Kelly[90] has also found this "free parameter" viewpoint useful in his linked-cluster studies of atomic structure.

Further study of this cancellation argument leads to two important conclusions.[9] First, the convergence of the *energy* expansion is not the most useful criterion for choosing the shell-model potential. There are serious "overcounting problems" associated with the higher-order terms in the energy expansion, and these can lead to ambiguities in the choice of insertions to be included in V_{SM}. These overcounting problems disappear if one considers instead the expansion for the true expectation value $\langle \mathcal{O} \rangle$ of some operator $\mathcal{O}$. This argument leads one to the *same* choice of V_{SM} for *any* operator $\mathcal{O}$. We thereby conclude that the choice of V_{SM} should optimize the rate of convergence for the *total wave function*. The second conclusion is that the best rate of convergence is obtained when the various linked-cluster terms are arranged according to their on- or off-energy-shell properties. The result is that the shell model potential should be defined by the sum of all single-particle insertions which can be placed *entirely* on the energy shell by means of g.t.o. factorizations. Quite fortunately, this choice of V_{SM} includes *all* of the insertions which connect occupied and unoccupied states. The generalized Brillouin condition can therefore be satisfied exactly. This is a very useful simplification. It also has a rather curious side effect. The matrix elements $\langle b' \mid V_{\mathrm{SM}} \mid b\rangle$ are essentially zero, and therefore the orbitals ϕ_b are essentially just plane waves. But this cannot be completely true, because plane waves are not orthogonal to the occupied orbitals ϕ_m. The "particle–hole" matrix elements $\langle m \mid V_{\mathrm{SM}} \mid b\rangle$ are *not* negligible, however, and these distort the ϕ_b's in such a way as to preserve the orthogonality condition.

There is still, however, one formal difficulty. This definition of V_{SM} is not yet completely Hermitian. The single-particle energies are all real, but the orbitals are not all mutually orthogonal. A Hermiticity problem of this type was first solved by Balian and DeDominicis,[119] in the context of their "quasi-particle" formulation of quantum statistical mechanics. Another approach, which appears more convenient for the nuclear problem, is indicated here at the end of Appendix D. With this modification, the diagram cancellation argument is seen to provide a quite satisfactory definition for the shell-model potential.

Variational Principle

This definition of V_{SM} is completely perturbation-theoretic. It makes no reference to any variational

[117] R. K. Nesbet, Phys. Rev. **109**, 1632 (1958).
[118] P.-O. Löwdin, J. Math. Phys. **3**, 1171 (1962).
[119] R. Balian and C. DeDominicis, Physica **30**, 1927 (1964).

principle. Nevertheless, one expects a nucleus to be stable against deformations away from its ground-state equilibrium configuration. Stability arguments have played a very important role in theories of collective motion, and a "fundamental" theory of nuclei ought to establish contact with this work. This can best be done by means of a variational principle.

There is another reason for desiring a variational formulation of the theory. It is extremely tedious to carry out fully self-consistent calculations of nuclei.[4] On the other hand, harmonic oscillator orbitals are quite convenient to work with, and it is well known that these are a rather good approximation for the occupied states of the lighter nuclei. One expects the use of oscillator orbitals to cause very little error in the total binding energy. Furthermore, one expects that the optimum value for the oscillator well parameter can be found by minimizing the total energy. A number of calculations have been based on these assumptions.[5–7,12,13] If this approach is to make sense, it is obviously very important to demonstrate that the expression used to calculate the total energy, for a "trial" set of occupied orbitals, should go through a minimum (or at least a stationary point) when these orbitals coincide with those of a fully self-consistent calculation. A stationary prescription for the total energy should also clear up any ambiguities in the choice of single-particle energies (which enter in the G-matrix calculations), as well as the proper form for the intermediate state orbitals. We have argued above that the Raleigh–Ritz principle is not able, by itself, to settle these questions. But it is not too much to ask that the perturbation theory should be *consistent* with the Raleigh–Ritz principle.

The *complete* expansion must naturally give an energy independent of the assumed form of $H_0=T+V_{\mathrm{SM}}$. The real problem is therefore to demonstrate that the linked expansion can be terminated in ways which have the desired stationary property. The full demonstration is rather long, and will be given elsewhere. But the basic idea is simple enough, as we shall now show.

Suppose that one performs a fully self-consistent calculation in the presence of a fictitious external potential, using

$$H_0'=T+V_{\mathrm{SM}}'+V_{\mathrm{ext}}, \tag{10.1}$$

$$V=v-V_{\mathrm{SM}}'. \tag{10.2}$$

The external potential is a Hermitian one-body operator, presumably rather weak but otherwise quite arbitrary. The term V_{SM}' is *not* arbitrary. It is "self-consistent" in the perturbation theoretic sense described above. That is, it consists of all on-energy-shell insertions. It has the virtue of satisfying the generalized Brillouin condition *in the presence of* V_{ext}. This is useful because it justifies the neglect of any single-particle excitations which might otherwise arise from the lack of *true* ($V_{\mathrm{ext}}\equiv 0$) self-consistency. [Any deviations from true self-consistency may be attributed to V_{ext}. One can always estimate the lack of true self-consistency by straightforward perturbation methods, but there is no point in doing this until *after* the "best" variational wave function has been found.]

This V_{SM}' must depend on V_{ext}, but this is not really a significant complication. The whole argument is really a "gedanken" one. We merely assume that this problem is well-defined, and that it can be solved in principle. We then assume that the "inverse" problem is also well-defined. By this, we mean that for any "trial" set of occupied orbitals $\{\phi_m\}$, which are orthonormal and reasonably close to the true ones, there should exist *some* V_{ext} for which this "trial" set emerges as the self-consistent solution.

Now consider the total wave function Ψ' which emerges from this calculation. This can be used to calculate a *fictitious* expectation value $\langle H\rangle'$ for the *true* Hamiltonian $H=T+v$. Since the "wrong" wave function is being used here, the Raleigh–Ritz principle says that

$$\langle H\rangle'\geq E_{\mathrm{true}}. \tag{10.3}$$

The variational parameters here are the "free parameters" within the Hermitian operator V_{ext}. For practical purposes, we assume that the "trial" orbitals ϕ_m can be regarded instead as the independent parameters. (If the ϕ_m's are varied independently, Lagrange multipliers will be needed to preserve orthonormality.) A general variation of V_{ext} also allows for independent variations of the single-particle energies E_m, E_b. These degrees of freedom are not useful here. It is best to use the optimum values for these E's as given by the stationary condition. This corresponds to the case $V_{\mathrm{ext}}=0$, showing that it is best to use just the usual self-consistency definition (see Ref. 9) for these E's.

There are two parts to the proof that this variational argument is really applicable to the perturbation theory of nuclei outlined above. First, it must be shown that the "trial" expectation value,

$$\langle H\rangle'\equiv\langle\Psi'\,|\,H\,|\,\Psi'\rangle/\langle\Psi'\,|\,\Psi'\rangle, \tag{10.4}$$

is equivalent to the type of energy expression one actually uses in nuclear calculations. The latter is a "model" type expression [see (9.20), (9.21)], in the sense that $E=E_0+\Delta E$. But the infinite partial summations lead to overcounting problems. When this overcounting is corrected for by appropriate subtractions, one ends up with the "renormalized" energy expression described in Ref. 9. It was found that this new energy expression satisfies a very remarkable "mass operator variational principle". The proof of the present variational argument (to be given elsewhere) amounts to demonstrating that our external potential argument is really the correct physical interpretation

for this rather mysterious looking variational principle.[120]

The second task is to show that one can obtain similar variational principles, or "stationary approximations" for the total energy, when the complete expansion is terminated. This is very easy. Similar mass operator variational principles hold for *any* selection of skeleton diagrams. It is only necessary that these skeletons be used *consistently* in all parts of the formalism: in the main energy term (the $\mathfrak{D}$ of Ref. 9), in the true occupation probabilities P_m [see (9.11)], and in the "mass operator" insertions which define V_{SM}. (Note that V_{SM} is needed to define the single-particle energies E_m, even when the ϕ_m's are given. Any differences between these ϕ_m's and a fully self-consistent basis should be attributed to V_{ext}.) Any choice of skeletons will lead to a "stationary approximation". Obvious choices are to consider only two-body correlation terms [as in (9.11)], or only two- and three-body terms. These approximations will be discussed elsewhere.

Open-Shell Nuclei

In the case of open-shell atoms, the Hartree–Fock theory is not uniquely defined. Roothaan[121] and Bremond[122] have both used the variational approach, (a) above, to extend the Hartree–Fock theory to rather special cases of degeneracy. The so-called Hartree–Bogolubov method[123] is another extension of the theory, designed to include effects of pairing correlations. But we have not seen any general discussion of the open-shell problem.

The diagram cancellation argument, (c) above, is especially useful here because of its inherent flexibility. There is no one "best" definition of V_{SM} for all open-shell nuclei. We shall mention three types of possibilities: (I) If the ratio (n/N) of the numbers of valence and core particles is small enough, one can put *all* the particles in the self-consistent V_{SM} obtained from the nearest closed-shell nucleus. By treating *all* effects of the valence particles as perturbations, one can take full advantage of the formal separation between core and valence effects achieved by Bloch and Horowitz.

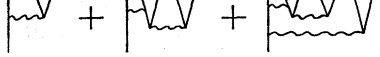
If, on the other hand, the valence-induced core deformations are too large to handle as perturbations, one should make some allowance in V_{SM} for both the "field-producing" and "exclusion" effects of the valence particles. (Examples of these effects are shown below.) This will naturally tend to spoil the clean separation of core and valence effects, since the core terms will now include, through V_{SM}, part of the valence effects. [Very high-order repetitions of one-body insertions would remove these valence effects from the core terms, if only the core-particle contributions to these insertions are considered. But, as shown below, the valence diagrams include terms consisting of core skeleton diagrams with insertions involving valence particles. V_{SM} can be chosen to cancel both the core and the valence-particle contributions to these insertions.] One way of treating these effects is to (II) define V_{SM} for for some "average" nuclear eigenstate, in effect averaging over the multiplet structure of certain low-lying eigenstates.[121,124] The Nilsson model belongs in this category. Finally, one could (III) devise schemes whereby V_{SM} optimizes the treatment of some particular eigenstate.

These problems lie in the domain of conventional shell-model theory—nuclear matter theory really has very little to add here. In this connection the linked expansions should simply be regarded as a "bookkeeping system," without any implications as to whether the core deformations should be treated by perturbation methods or by "self-consistent" methods. Nevertheless, the higher-order correction terms will always remain well-defined for any reasonable choice of V_{SM}.

In any event, it may be helpful to see just how these core deformation effects appear in the present formalism. We have seen that the total wave function can be written in the exponential form

$$\Psi = \exp\left(\sum_r \mathbf{Y}_{Lr}\right) \exp\left(\sum_s \mathbf{W}_s\right) |\Psi_D\rangle, \quad (7.30)$$

where the "folded, linked, open valence parts" $\mathbf{Y}_{Lr}$ were obtained by applying the reduction (5.18) to the bottoms of the $\mathbf{Y}_r$'s of Sec. VI, and then "folding in" the reduced $\mathcal{U}_V$'s of Sec. V. Among these $\mathbf{Y}_{Lr}$'s there will be terms of the form



$$+ \cdots \quad , \quad (10.5)$$

corresponding to

$$\exp(\Delta\mathbf{W}), \quad (10.6)$$

where $\Delta\mathbf{W}$ represents all the modifications of $\sum_r \mathbf{W}_r$ brought about by the effects of the valence particles. Their characteristic feature, which distinguishes them from other $\mathbf{Y}_{Lr}$ correlations, is that the valence particles remain within the band of valence orbitals after their interactions with the core. The terms shown in (10.5)

[120] This idea of using an auxiliary external potential has been widely used in statistical mechanics. The subject is reviewed, from the perturbation viewpoint, by C. Bloch in Ref. 38.

[121] C. C. J. Roothaan, Rev. Mod. Phys. **32**, 179 (1960).

[122] B. Bremond, Nucl. Phys. **58**, 687 (1964).

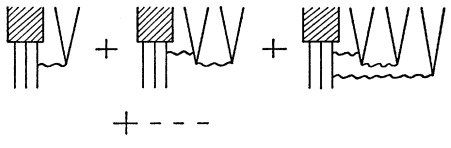
[123] N. N. Bogoliubov, Soviet Phys.—Usp. **2**, 236 (1959); J. G. Valatin, Phys. Rev. **122**, 1012 (1961); M. Baranger, Phys. Rev. **122**, 992 (1961); and **130**, 1244 (1963); M. Baranger, in 1962 *Cargese Lectures in Theoretical Physics*, M. Levy, Ed. (W. A. Benjamin, Inc., New York, 1963).

[124] I. Kelson and C. A. Levinson, Phys. Rev. **134**, B269 (1964); W. H. Bassichis, C. A. Levinson, and I. Kelson, Phys. Rev. **136**, B380 and B385 (1964); W. H. Bassichis, B. Giraud, and G. Ripka, Phys. Rev. Letters **15**, 980 (1965); M. K. Pal and A. P. Stamp, Phys. Rev. **158**, 924 (1967). A critique of this approach has been given by H. G. Benson and J. M. Irvine, Proc. Phys. Soc. (London) **89**, 249 (1966).

are all of the "field-producing" type. There will also be some exclusion corrections with a very similar form, as shown in (10.7). [This should be compared with (5.16d).]

(10.7)

There will also be "mixed" terms of the form

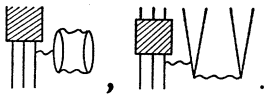


(10.8)

which correspond to

$$\exp(\mathbf{Y}_L{}^0)\exp(\Delta \mathbf{W}), \tag{10.9}$$

where $\mathbf{Y}_L{}^0$ represents the terms in the operator $\sum_r \mathbf{Y}_{Lr}$ which do *not* contain any of these core deformation effects. Finally, there will be some "mixed" terms which are not completely open, such as



(10.10)

[In all of these diagrams we have simply shown the principal parts. The "external" lines at the bottom may also attach to some "folded in" insertions. Thus, the first diagram in (10.10) is actually cancelled by a similar folded diagram.] These terms combine in obvious ways to give the changes in ΔE and $\langle \alpha \mid \mathcal{O} \mid \beta \rangle$ resulting from the core deformations.

XI. SUMMARY AND CONCLUSIONS

The time and temperature-independent linked-cluster expansions (for energy, wave function, and general expectation value, both for nondegenerate and degenerate systems) have been discussed from a unified and elementary viewpoint. Starting with the Brillouin–Wigner perturbation theory, the interaction energy terms ΔE have been expanded out of the energy denominators. The resulting series have then been rearranged to demonstrate the cancellation of unlinked terms.

This algebraic approach has the advantage of avoiding artificial limiting processes (adiabatic or thermodynamic) which are not essential for an understanding of ground and low-lying nuclear states. For this reason, and because one deals right from the beginning with the desired quantities ΔE and Ψ, this method is very convenient for settling questions of physical interpretation. We have examined the way these expansions express such "physical" features as antisymmetry, self-energy effects, wave-function renormalizations, and the relations between "true" and "model" single-particle occupation numbers. The exclusion-violating terms were seen to play several important roles. The relative merits of linked-cluster and ordinary Brillouin–Wigner methods, for few-body systems such as light nuclei, have been considered. The problem of defining the shell-model potential has also been carefully discussed.

These expansions are seen to form an extremely powerful and flexible set of tools. In principle, they are capable of handling *any* bound-state problem in nuclear structure where time-dependence and elementary-particle aspects do not enter explicitly. The possibility of extending these methods to time-dependent problems, such as nuclear reactions, was also discussed. The close connections between these expansions and modern shell-model concepts should also be stressed. They express most results in terms of the convenient "model" quantities: model energies, model wave functions, and effective interactions. Furthermore, the Bloch–Horowitz formalism reveals the full generality of a phenomenon frequently observed—the main effect of high-lying configurations is to simply "renormalize" the effects of the low configurations.

The analogies between these results and the Landau theory of Fermi liquids have been emphasized and exploited. It appears quite possible that these methods may converge rapidly enough to be useful also for liquid He^3 calculations.

In any application, of course, one must pay careful attention to the delicate problems of convergence. These are asymptotic expansions, and they are bound to diverge in the strict mathematical sense. The most obvious divergences can be traced to two sources: (a) singularities in the interaction, and (b) quasi-degeneracy, i.e., strong admixtures of certain low-lying states. (These strong admixtures can be thought of as "phase transitions.") Against these difficulties the formalism provides several weapons, namely partial summations and the great freedom of choice for H_0 and the quasi-degenerate subspace D (the "model subspace"). After eliminating the obvious divergences, we feel that one should not be unduly concerned about the use of asymptotic expansions. Experience shows that there are two dangers to guard against. One is that the "phase transitions" may not be very obvious, as in the famous BCS example, and also in the case of nuclear deformations. The other is that further partial summations may be required,[11,9] because of subsets of individually finite terms which nevertheless form divergent series.

Finally, we should emphasize that it is not enough to simply eliminate divergences, or even to obtain "reasonable looking" expressions. It is important to study the remaining higher-order terms, to determine as well as possible whether these can cause significant changes or "renormalizations" of the numerical results.

This has been one of the main motivations for the present study.

ACKNOWLEDGMENTS

It is a pleasure to thank Ben Day for discussions about his derivation of the Bloch–Horowitz expansion, and also to thank R. Rajaraman and Professor C. Bloch for important clarifications of the diagram rules. I am deeply grateful to Professor Bethe for encouraging this study, and for helpful advice. I would also like to thank Professor G. E. Brown and his coworkers, especially A. M. Green and C. W. Wong, for many stimulating conversations about practical applications of diagrammatic methods in nuclear structure studies, and to thank Dr. C. DeDominicis and Dr. R. Balian for an introduction to their very elegant renormalization methods. Thanks are due also to E. Østgaard and G. E. Brown for informing me of their recent investigations of liquid He^3. It is a pleasure to thank Professor Aage Bohr and the other members of the Niels Bohr Institute for their very kind hospitality during a large part of this work. Financial support from the National Science Foundation is gratefully acknowledged.

APPENDIX A

Analytic Properties of the Secular Matrix

Bloch and Horowitz[44] have studied the analytic properties of the secular matrix (2.14) for complex E. This appendix discusses the more important properties from a simple viewpoint.[125] Let a and b be general noncommuting matrices. The identity

$$(a-b)^{-1}-a^{-1}=a^{-1}a(a-b)^{-1}-a^{-1}(a-b)(a-b)^{-1}$$
$$=a^{-1}b(a-b)^{-1} \tag{A1}$$

may be iterated to give the well-known result

$$(a-b)^{-1}=\sum_{n=0}^{\infty}(a^{-1}b)^n a^{-1}=a^{-1}\sum_{n=0}^{\infty}(ba^{-1})^n. \tag{A2}$$

This can be used twice to obtain

$$(a-b-c)^{-1}=(a-b)^{-1}\sum_{m=0}^{\infty}[c(a-b)^{-1}]^m$$
$$=\sum_{l=0}^{\infty}(a^{-1}b)^l a^{-1}\sum_{m=0}^{\infty}[c\sum_{n=0}^{\infty}(a^{-1}b)^n a^{-1}]^m$$
$$=\sum_{l=0}^{\infty}(a^{-1}b)^l\sum_{m=0}^{\infty}[a^{-1}c\sum_{n=0}^{\infty}(a^{-1}b)^n]^m a^{-1}. \tag{A3}$$

With the identifications

$$a=z-H_0, \qquad b=QV, \qquad c=PV, \tag{A4}$$

P and Q being projection operators on and off the model subspace, (A3) becomes

$$(z-H)^{-1}=\Omega\sum_{m=0}^{\infty}[(z-H_0)^{-1}P\mathcal{U}(z)]^m(z-H_0)^{-1}$$
$$=\Omega[z-H_0-P\mathcal{U}(z)]^{-1}. \tag{A5}$$

We have identified the summation in (A2) with Ω, regarding this as the iterative solution of (2.11). Multiplying on both sides by P gives

$$P(z-H)^{-1}P=P[z-H_0-P\mathcal{U}(z)]^{-1}P. \tag{A6}$$

For any state vector Ψ_D lying entirely within the degenerate subspace, we therefore find

$$\sum_{n=0}^{\infty}\frac{|\langle\Psi_n|\Psi_D\rangle|^2}{z-E_n}=\sum_{j=1}^{d}\frac{|\langle\Psi_j(z)|\Psi_D\rangle|^2}{z-\lambda_j(z)}, \tag{A7}$$

where Ψ_n and E_n are the exact eigenstates and eigenvalues. Here $\Psi_j(z)$ and $\lambda_j(z)$ are (normalized) solutions of the d-dimensional eigenvalue problem

$$P[H_0+\mathcal{U}(z)]P\Psi_j(z)=\lambda_j(z)\Psi_j(z). \tag{A8}$$

Given any Ψ_D, both sides of (A7) become ordinary complex functions of z, thus both sides must share the same analytic properties. In particular, the poles must be the same, which shows that every solution of

$$z=\lambda_j(z), \qquad 1\leq j\leq d \tag{A9}$$

must be real and equal to some exact eigenvalue E_n. The set of solutions to (A9) must, in fact, be identical to the set of eigenvalues E_n.

The factors $(1/a)$ in (A3) are all nonsingular and well-defined matrices when z is nonreal. We therefore regard this resolvent-kernel formalism as a useful tool for analytically continuing $\mathcal{U}(z)$ beyond the radius of convergence of its perturbation expansion. Having thus defined $\mathcal{U}(z)$ for all z, we may now restrict the discussion to z's on the real axis. For any *fixed and real* z, $\mathcal{U}(z)$ becomes a Hermitian matrix, so the set of $\Psi_j(z)$'s can be considered orthonormal. (For nonreal z the Ψ_j's are not necessarily orthogonal; thus the numerators on the right-hand side of (A7) must actually involve bi-orthogonal vectors, as discussed in Appendix D. This cannot affect the poles, since these are all real and can be approached entirely through real values of z.)

Let Ψ_{Dn} be a multiple of the degenerate projection of Ψ_n, such that Ψ_n and Ψ_{Dn} are both normalized to unity. The residue of the left-hand side of (A7) at $z=E_n$ is then the overlap $|\langle\Psi_n|\Psi_{Dn}\rangle|^2$. Only one term (call this n) of the j summation will be large, when $z\approx E_n$, thus the right-hand side approaches $[z-\lambda_n(z)]^{-1}$ and its residue must be $[1-\lambda_n'(E_n)]^{-1}$. This shows that if the norm of Ψ_n is increased until $\langle\Psi_n|\Psi_{Dn}\rangle=1$ (the usual condition in *BW* perturbation theory), then

$$\langle\Psi_n|\Psi_n\rangle=1-\lambda_n'(E_n). \tag{A10}$$

[125] Thanks are due to Ben Day for suggesting the use of resolvent kernels for this discussion.

We now observe that for real z,

$$\lambda_j'(z) = \langle \Psi_j' \mid H_0 + \mathfrak{V} \mid \Psi_j \rangle + \langle \Psi_j \mid \mathfrak{V}' \mid \Psi_j \rangle + \langle \Psi_j \mid H_0 + \mathfrak{V} \mid \Psi_j' \rangle = \langle \Psi_j \mid d\mathfrak{V}/dz \mid \Psi_j \rangle + \lambda_j (d/dz) \langle \Psi_j \mid \Psi_j \rangle. \quad \text{(A11)}$$

The last term vanishes because the Ψ_j's are defined to have unit norm for all z. Finally, we note that $\langle \mathfrak{V}' \rangle$ is always negative, so that (A10) is always larger than unity. It is interesting to compare this general BW result with the "valence" normalization factors (6.21) for the BH expansion.

Bloch and Horowitz have also pointed out that the matrix elements of $\mathfrak{V}(z)$ have simple poles situated on the real axis. [These can generally be related to zeroes on the left-hand side of (A7).] From the general structure of the $\mathfrak{V}$ perturbation expansion [see especially (2.7)], one would expect these poles to be located near the unperturbed energies E_i of the "nondegenerate" states Φ_i, provided that "self-energy" terms in the expansion have been properly identified and included in H_0. This suggests a poor rate of convergence for those eigenstates whose energies E_n lie close to "nondegenerate" unperturbed energies E_i. The remedy obviously lies in the proper choice of degenerate subspace.

APPENDIX B

Diagram Rules

The following list expresses the Goldstone diagram rules in an unambiguous form convenient for nuclear applications.

(i) Draw *just one diagram* from the set of all those obtained from each other when "direct" interactions are replaced by "exchange" interactions, or vice versa. Disregard all other members of this "exchange group." (It is usually convenient to choose a diagram with the maximum possible number of closed loops.)

(ii) Include a factor of $(\frac{1}{2})$ for each "equivalent pair" of lines. Two lines form an equivalent pair if they (1) both begin at the same interaction, (2) both end at the same interaction, and (3) both go in the same direction.

(iii) Include an over-all sign factor of $(-1)^{l+h}$, where l is the number of closed loops and h the number of downgoing or "hole" line segments.

(iv) Replace each matrix element of v or G by a "direct minus exchange" element (an element of the form $\langle ij \mid v \mid kl-lk \rangle$), where the original element is to be considered "direct".

(v) Include the energy denominators, given by the sum of all downgoing line energies minus the sum of all upgoing line energies.

(vi) Sum each upgoing line *independently* over all particle states (b states), and each downgoing line *independently* over all hole states (m states). The exclusion-violating terms which arise from these independent summations must all be included.

These rules represent a combination of those given by Goldstone[28] and Hugenholtz.[29] The present formulation has several advantages. In the first place, Hugenholtz's "equivalent pair" rule is much clearer than Goldstone's original statement that one should sum over "all distinct possibilities." This avoids much confusion in higher-order terms. Secondly, we prefer Goldstone's diagrams over those of Hugenholtz; thus interactions are represented by lines, instead of by dots (even though each line now represents a "direct minus exchange" matrix element), because there is less chance of confusion over minus signs. Nevertheless, it may be helpful to think in terms of Hugenholtz's "dot" diagrams while assigning complicated Goldstone diagrams to their respective exchange groups.

Finally, we should emphasize the advantages of always working with "direct minus exchange" elements. One is forced, when dealing with realistic nuclear forces, to expand all the elements in partial waves. This is due both to the strong spin dependence of the forces, and to the nature of available methods for solving the Bethe–Goldstone equation. After expanding the "direct" matrix elements in terms of (L, S, T, J) eigenstates, the effect of including exchange terms is simply to double the weight of states with "allowed" (S, T, parity) quantum numbers, and to eliminate the "unallowed" states. This shows that the main effect of antisymmetry (apart from the distinction between "particle" and "hole" states) is, *to all orders of perturbation theory*, the same as simply replacing the original interaction,

$$v = \sum_{LSTJ} v_{LSTJ} P_{LSTJ}, \quad \text{(B1)}$$

by a "direct minus exchange" interaction,

$$v_{D-E} = 2 \sum_{\text{allowed}(LSTJ)\text{'s}} v_{LSTJ} P_{LSTJ}, \quad \text{(B2)}$$

where the P's are projection operators. Since these P's must be introduced anyway for realistic nuclear forces, it is no more difficult to calculate all 2^n numbers of an nth order "exchange group", i.e., a Hugenholtz diagram with n "dots," than to calculate a single member.

It is interesting to see how these rules apply to an upgoing ladder of v interactions. Each intermediate state involves an equivalent pair, and thus a factor of $(\frac{1}{2})$. These cancel all but one of the factors of 2 from (B2), the net result being simply that each "direct" G-matrix element is replaced by a "direct minus exchange" element. The diagram rules, as well as the statement concerning (B1) and (B2), are therefore all valid for the expansion in reaction matrices G. This agrees with the intuitive argument that the G-matrix and v-matrix expansions should become indistinguishable in the limit of weak interaction.

Spin summations require some care, when dealing with spin-dependent forces such as (B1), (B2). These summations can always be carried out by means of a trace formalism, in close analogy to the way spins are treated in quantum electrodynamics. Individual single-particle states are labelled (in nuclear matter) by their spin projections (s_3, t_3), while the interactions involve projection operators such as $P_{S=1}=\frac{1}{4}(3+\vec{\sigma}_1\cdot\vec{\sigma}_2)$. One can therefore always reduce spin sums to traces of products of 2×2 Pauli matrices.[126]

A complete derivation of the rules is quite tedious. Many of the details are discussed in references 28, 29, 38, and 42. We shall simply offer some hints here for the reader who wishes to work them out for himself. The usual discussion of Wick's theorem leads to the statement that one should sum over "all topologically distinct graphs." This is not concise enough to give the rule about equivalent-pair factors of $(\frac{1}{2})$. The reader is encouraged to work out the first three orders,

$$\langle\Phi_0\mid V,\ V^2,\ V^3\mid\Phi_0\rangle,$$

directly in terms of the Fermion operators, starting with (4.2) and

$$\mid\Phi_0\rangle=(\prod_{m=1}^{N}\eta_m{}^\dagger)\mid 0\rangle,$$

where $\mid 0\rangle$ is the absolute vacuum. This should demonstrate the convenience of collecting together all members of an exchange group and treating them all simultaneously. This should also clarify the $(-1)^{l+h}$ rule.

The next step is to verify the equivalent-pair rule for a rather simple case, the nth-order "upgoing ladder" diagram.[127] (This is the v^n term in the lowest-order diagram of the reaction-matrix expansion.) The n factors of $(\frac{1}{2})$, coming originally from (4.2), remain intact after one notes that $\sum_{l<m}=\frac{1}{2}\sum_{l,m}$ and that $\langle lm-ml\mid V\mid ab-ba\rangle=2\langle lm\mid V\mid ab-ba\rangle$. (It is easiest to think of *distinct* pairs of occupied states l, m, and to convert to unrestricted summations $\frac{1}{2}\sum_{l,m}$ only in the final step.) Note also that there are n equivalent pairs in this diagram. Now consider an $(n+1)$th-order diagram obtained from the previous ladder by adding a single $(-V_{\rm SM})$ insertion [see (4.2)] at some intermediate level. This will necessarily be attached to one member or the other of a pair of lines (a, b or l, m) that was previously "equivalent". These two lines are distinct, before summing over a, b or l, m, so two distinct diagrams can be obtained by attaching $(-V_{\rm SM})$ to this pair. After the summation, however, these diagrams become identical; therefore only one of these "topologically equivalent" diagrams need be considered if the corresponding equivalent-pair factor of $(\frac{1}{2})$ is also dropped. This argument is easily extended to a general diagram. Consider the effect of each successive interaction, proceeding "timewise" from the bottom to the top of the diagram. One loses a factor of $(\frac{1}{2})$ every time an interaction destroys the equivalence of a pair.

[126] T. Dahlblom, K.-G. Fogel, B. Qvist, and A. Törn, Nucl. Phys. **56**, 177 (1964).

[127] I am indebted to R. Rajaraman for greatly clarifying this argument.

Bloch–Horowitz Diagrams

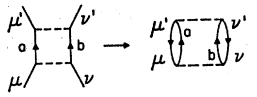
Some additional rules are required for the valence diagrams of the Bloch–Horowitz expansion. The main problem is to obtain the correct over-all sign factors. First of all, it is necessary to choose a "standard order" for the set of valence states. (This determines the phases of the model determinants Φ_i.) Then a convenient prescription is:

(i′) Pull the *ends* of the external lines across each other to bring the valence-state labels into standard order, both at the top and bottom of the diagram.

(ii′) Wrap each diagram around a transparent horizontal cylinder, and connect together the ends of the external lines at the back of the cylinder. The standard order must be observed in forming these connections, i.e., the "first" line from the top must be joined to the "first" line from the bottom, etc., even though their actual labels may be different. These new diagrams should now look like Goldstone diagrams. The over-all sign is now given by the usual $(-1)^{l+h}$ rule.

(iii′) Apply the rules given above for the Goldstone diagrams, with the following obvious modifications: (a) the "external" valence lines (those which were originally external) must not be summed over, (b) the equivalent-pair rule must not be applied to these lines, and (c) the energy denominators are now given by (5.23), where the "upgoing" and "downgoing" lines refer to the original external-line diagrams.

For the *external* lines of each diagram belonging to a particular matrix element $(v_V)_{ij}$, one must eventually consider all permutations of the distinct valence states belonging to Φ_i and Φ_j. As an example, consider the $n=2$ diagram shown in (B3).



(B3)

(We have assumed here that $\mu<\nu$, $\mu'<\nu'$.) The sum of all diagrams in this "exchange group" is

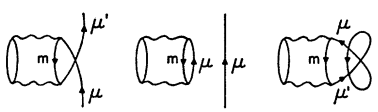
$$\tfrac{1}{2}\sum_{ab}\langle\mu'\nu'\mid v\mid ab-ba\rangle[E_V-(E_a+E_b)]^{-1}\langle ab\mid v\mid\mu\nu-\nu\mu\rangle,\quad\text{(B4)}$$

where the factor $(\frac{1}{2})$ is due to the single equivalent pair a, b.

Two more qualifications are necessary. First, the upgoing internal lines are to be summed over all μ states as well as all b states, subject to one restriction. The Q operator in (2.7), (2.12) forbids all many-body intermediate states Φ_i which lie within the degenerate

subspace, thus at each intermediate level there must be at least one particle in a b state, or at least one hole in an m state. When this restriction involves an equivalent pair, the factor $(\frac{1}{2})$ is to be retained only if one restricts first one member of the pair, and then the other, to b states, summing the "other" member over the μ states in each case.

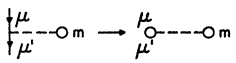
Secondly, there is a question of interpretation for certain of the diagrams. Consider diagram (a) of (B5), which includes the exchange correction for term (b) of the original BW expansion.



(B5)

To find the required factor of (-1), we follow rule (ii') above and obtain diagram (c). The familiar $(-1)^{l+h}$ rule still applies, but one must now interpret the (m, μ, μ') loop as "two holes and one loop."

Finally, we consider the changes required by the "valence-hole" description, where the degenerate states Φ_i are labelled by n' valence holes as well as n valence particles. The $\mathcal{U}_V$ diagrams will now have n' *downgoing* external lines, in addition to n upgoing external lines. Two minor changes are required. First, the valence hole states must also be given a "standard order", and the ends of the external hole lines must be connected according to this ordering. Secondly, the number of hole line segments, *including* the external line segments, must be counted *before* wrapping the diagram around the cylinder. The n holes which result from joining the n external particle lines should then be added to this number, to give the final h for the sign factor $(-1)^{l+h}$. In other words, the "wrapping" of an external particle line must *always* increase h by unity [see the discussion of diagram (c) above], whereas the wrapping of an external hole line creates an upgoing line segment which does not contribute to h. Remember that an external hole line which interacts only once will have *two* segments, thus the contribution of (B6)



(B6)

is

$$-\sum_m \langle \mu' m \mid v \mid \mu m - m\mu \rangle. \tag{B7}$$

(Note also the location of the labels μ and μ'.) The internal hole lines should be summed, independently, over all m states, except for the restriction that there must not be any quasi-degenerate states among the many-body intermediate states of $\mathcal{U}_V$.

Rules for the linked expansion of $\mathcal{U}_V$ are given in Sec. VII.

APPENDIX C

Magnitudes of Linked Diagrams

We wish to demonstrate[128] that for large saturating systems, the ΔE contribution of every Goldstone diagram is proportional to N. Consider a system of large volume Ω, where one can assume momentum conservation. Neglect spins, and assume a two-body interaction, v, characterized by depth v_0 and range a. Then

$$\phi_j = \Omega^{-1/2} \exp(i\mathbf{k}_j \cdot \mathbf{r}), \tag{C1}$$

$$\langle ij \mid v \mid kl \rangle \sim v_0 a^3 \Omega^{-1} \delta^3_{\mathbf{k}_i + \mathbf{k}_j, \mathbf{k}_k + \mathbf{k}_l}, \tag{C2}$$

$$\sum_{j<k_F} \sim N = \rho\Omega, \tag{C3}$$

and

$$\sum_{j<k_F} \sim \Omega a^{-3}. \tag{C4}$$

The last of these relations comes from the fact that intermediate state momenta are typically of order a^{-1} for an interaction of range a.

Now consider an arbitrary linked diagram with n interactions and h holes. Note that:

(i) There are $2n$ lines altogether.

(ii) Momentum conservation imposes $(n-1)$ constraints among the various momenta of these $2n$ lines.

(iii) There are $2n-h-(n-1)=n+1-h$ momenta to be summed independently over states above the Fermi sea, giving a factor of order $(\Omega a^{-3})^{n+1-h}$.

(iv) Summation over the h hole states gives a factor of $N^h=(\rho\Omega)^h$.

(v) The n interactions contribute $(v_0 a^3/\Omega)^n$.

(vi) The $n-1$ energy denominators contribute $(1/e)^{n-1}$.

The total contribution of a linked (n, h) diagram is therefore of order

$$(v_0 a^3/\Omega)^n (e^{-1})^{n-1} (\rho\Omega)^h (\Omega/a^3)^{n+1-h} = N v_0 (v_0/e)^{n-1} (\rho a^3)^{h-1}. \tag{C5}$$

In (iii) and (iv), however, we have ignored the fact that momentum conservation sometimes restricts hole summations instead of particle summations. Each such restricted hole summation will remove a factor of (ρa^3).

The result is clearly proportional to N, since the Goldstone energy denominators do not contain ΔE and are independent of volume. Similar arguments show that a diagram with L linked parts is proportional to N^L. Note that the *energy per particle* is independent of Ω, which justifies the usual convention of ignoring all volume factors.

These arguments are easily extended to linked diagrams with a number x of pairs of external lines.[29] One

[128] W. B. Riesenfeld and K. M. Watson, Phys. Rev. **104**, 492 (1956).

finds that their magnitudes scale as N^{1-x}. For example, self-energy terms ($x=1$) are independent of N.

Let us see how these considerations are modified for the reaction-matrix expansion obtained by summing upgoing ladders of v interactions, if we now assume that v is a hard-core interaction of radius a. The factor v_0a^3 in (C2) is replaced by the core volume a^3, times a typical energy denominator e. The strength "v_0" is therefore replaced by e; thus (C5) becomes

$$N(\hbar^2/Ma^2)(\rho a^3)^{h-1}. \tag{C6}$$

This is independent of n, suggesting that the convergence in terms of G matrices might be very poor. This has led to a rearrangement of the expansion in which a "small parameter" can be clearly seen.[11,9] Naturally enough, this small parameter is essentially ρa^3.

APPENDIX D

Exact Forms for the Linked Valence Expansions, Hermiticity and Orthogonality

The linked-cluster results of Sec. VII are not all formally exact, even if convergence is assumed. The linked expansion for $\mathfrak{W}_\infty=\mathfrak{V}_{VL}$ and the "partially linked" form of N_V given in (7.25) are quite correct, but the exponential form of N_V, (7.29), and the expectation-value and transition-amplitude expressions (7.38) and (7.41) are somewhat incorrect. These contain errors arising from the matrix multiplications involving Θ. In effect, we have assumed the validity of the approximations

$$(\mathbf{A}_\beta^{(\alpha)\dagger}\Theta\mathbf{A}_\alpha^{(\alpha)})(\mathbf{A}_\alpha^{(\alpha)\dagger}\Theta\mathbf{A}_\alpha^{(\alpha)})^{r-1}\approx\mathbf{A}_\beta^{(\alpha)}\Theta^r\mathbf{A}_\alpha^{(\alpha)}\approx\delta_{\alpha\beta}(N_{V\alpha}-1)^r. \tag{D1}$$

These relations are inexact because Θ is actually diagonal only in the *nonorthogonal* basis $\mathbf{A}_\beta=\mathbf{A}_\beta^{(\beta)}\neq\mathbf{A}_\beta^{(\alpha)}$. Thus, if convergence or a valid analytic continuation is assumed,

$$\mathbf{A}_\beta^\dagger\Theta\mathbf{A}_\alpha\equiv\delta_{\alpha\beta}(N_{V\alpha}-1). \tag{D2}$$

This situation has been carefully analyzed by Des Cloizeaux.[55] His exact perturbation theory, when combined with the graphical methods of Sec. VII, leads to formally exact linked expansions for the physically interesting quantities. He replaces the nonorthogonal basis $\mathbf{A}_\alpha$ by a "natural" basis $\mathbf{A}_\alpha$ which is rigorously orthonormal. It turns out that the form of the transition amplitude matrix,

$$\mathfrak{M}=(\mathbf{I}+\Theta)^{-1/2}\odot(\mathbf{I}+\Theta)^{-1/2},$$

as expanded in (7.41), is actually exact, provided that the $\mathbf{A}_\alpha^\dagger$ and $\mathbf{A}_\beta$ of (7.33) are replaced by $\mathbf{A}_\alpha^\dagger$, $\hat{\mathbf{A}}_\beta$. The main problem is therefore to determine this natural basis. The correct procedure is to replace the non-Hermitian matrix $\mathfrak{W}_\infty$ by a symmetrized form of this matrix, denoted by $\mathfrak{K}$. The $\mathbf{A}_\alpha$'s are then the eigenvectors of this $\mathfrak{K}$. The actual form of this symmetrization is rather complicated, but it can be thought of as a generalization of the simple expedient $\mathfrak{W}\to\frac{1}{2}(\mathfrak{W}+\mathfrak{W}^\dagger)$. The information required for the construction of $\mathfrak{K}$ is contained, not too surprisingly, in the Θ matrix. As an introduction to this method, we first discuss some general properties of nonorthogonal vector systems.

At the end of this appendix we shall argue that a similar method can be used to restore the Hermiticity of the shell-model potential.

Natural Basis for a Nonorthogonal Vector System

The following discussion is based very closely on section 2 of Des Cloizeaux's paper.[55] Suppose we are given a set of d linearly independent vectors, $|\alpha\rangle$, which are not mutually orthogonal and which may (for the present) have arbitrary norms $n_\alpha=\langle\alpha|\alpha\rangle$. These vectors define a d-dimensional space D. Within this space we can always find a second set of d linearly independent (although not mutually orthogonal) vectors, $|\bar{\alpha}\rangle$, such that

$$\langle\bar{\beta}|\alpha\rangle=\langle\alpha|\bar{\beta}\rangle=\delta_{\alpha\beta}. \tag{D3}$$

These two sets, $|\alpha\rangle$ and $|\bar{\alpha}\rangle$, are said to form a *biorthogonal* vector system.

For example, let $\mathbf{A}_\alpha$ and $\bar{\mathbf{A}}_\alpha$ be the representations of $|\alpha\rangle$, $|\bar{\alpha}\rangle$ with respect to an orthonormal basis Φ_i for D: $\mathbf{A}_\alpha$=column vector $(a_{i\alpha})$, $\mathbf{A}_\alpha$=column vector $(\bar{a}_{i\alpha})$, where $|\alpha\rangle=\sum_i a_{i\alpha}|\Phi_i\rangle$, $|\bar{\alpha}\rangle=\sum_i\bar{a}_{i\alpha}|\Phi_i\rangle$. (The bar in $\bar{a}_{i\alpha}$ does *not* imply complex conjugation.) Then (D3), taken for all α's but with β fixed, gives an inhomogeneous set of d equations in d unknowns. These can always be solved to give $\mathbf{A}_\beta$ and hence $|\bar{\beta}\rangle$. For linearly independent $|\alpha\rangle$'s, the $|\bar{\alpha}\rangle$'s are always unique. This can be seen geometrically: The $d-1$ equations (D3) for $\alpha\neq\beta$ require that $|\bar{\beta}\rangle$ lie in the orthogonal complement of these $d-1$ vectors $|\alpha\rangle$. This orthogonal complement has just $d-(d-1)=1$ dimension, as is quite obvious for two and three-dimensional spaces D. Thus $|\bar{\beta}\rangle$ is constrained to lie along a definite axis. The last equation, $\langle\beta|\bar{\beta}\rangle=1$, then fixes its direction and length.

We now introduce a Hermitian operator

$$G\equiv\sum_\alpha|\bar{\alpha}\rangle\langle\bar{\alpha}|, \tag{D4}$$

which connects these two bases:

$$G|\alpha\rangle=\sum_\beta|\bar{\beta}\rangle\langle\bar{\beta}|\alpha\rangle=|\bar{\alpha}\rangle. \tag{D5}$$

Consider an arbitrary vector $|l\rangle$ in D. This can be expressed uniquely as

$$|l\rangle=\sum_\alpha\lambda_\alpha|\alpha\rangle, \tag{D6}$$

where λ_α is equal to $\langle\bar{\alpha}|l\rangle$. We see immediately that

$$\langle l|G|l\rangle=\sum_\alpha|\lambda_\alpha|^2>0, \tag{D7}$$

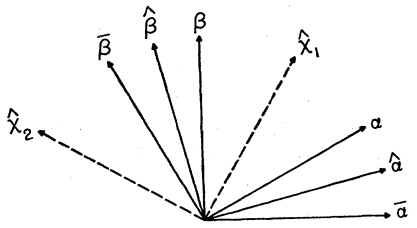


FIG. 3. Illustration of relations between the $|\alpha\rangle$, $|\bar{\alpha}\rangle$, and $|\hat{\alpha}\rangle$ bases. The "stretching axes" $|\hat{\chi}_1\rangle$ and $|\hat{\chi}_2\rangle$ are also shown. In this example $S_1<1$, $S_2>1$.

which demonstrates that G is positive definite. One consequence is that G has an inverse,

$$G^{-1}|\bar{\alpha}\rangle=|\alpha\rangle, \tag{D8}$$

which can be written as

$$G^{-1}=\sum_{\alpha}|\alpha\rangle\langle\alpha|. \tag{D9}$$

Now since G is Hermitian and positive definite, it must possess *d orthogonal* eigenvectors,

$$G|\chi_j\rangle=S_j|\chi_j\rangle, \tag{D10}$$

and its eigenvalues S_j must be real and positive definite. Geometrically speaking, G performs a simple stretching operation. We shall normalize the $|\chi_j\rangle$'s such that, together with the "parallel" set of vectors

$$|\bar{\chi}_j\rangle\equiv S_j|\chi_j\rangle, \tag{D11}$$

we have another bi-orthogonal system:

$$\langle\chi_i|\bar{\chi}_i\rangle=\langle\bar{\chi}_i|\chi_j\rangle=\delta_{ij}. \tag{D12}$$

This obviously requires that

$$\langle\bar{\chi}_j|\bar{\chi}_j\rangle=(\langle\chi_j|\chi_j\rangle)^{-1}=S_j. \tag{D13}$$

It is also convenient to introduce an orthonormal basis,

$$|\hat{\chi}_j\rangle=S_j^{1/2}|\chi_j\rangle=S_j^{-1/2}|\bar{\chi}_j\rangle. \tag{D14}$$

Thus we can write

$$G=\sum_j|\hat{\chi}_j\rangle S_j\langle\hat{\chi}_j|=\sum_j|\bar{\chi}_j\rangle\langle\bar{\chi}_j|, \tag{D15}$$

and

$$G^{-1}=\sum_j|\hat{\chi}_j\rangle S_j^{-1}\langle\hat{\chi}_j|=\sum_j|\chi_j\rangle\langle\chi_j|. \tag{D16}$$

When the eigenvalues S_j are all nondegenerate the $|\hat{\chi}_j\rangle$'s will be uniquely defined, apart from trivial phase factors which have no influence in the following developments.

We now introduce the "square-root" matrices,

$$G^{1/2}=\sum_j|\hat{\chi}_j\rangle S_j^{1/2}\langle\hat{\chi}_j|=\sum_j|\hat{\chi}_j\rangle\langle\bar{\chi}_j|$$
$$=\sum_j|\bar{\chi}_j\rangle\langle\hat{\chi}_j|, \tag{D17}$$

and

$$G^{-1/2}=\sum_j|\hat{\chi}_j\rangle S_j^{-1/2}\langle\hat{\chi}_j|=\sum_j|\hat{\chi}_j\rangle\langle\chi_j|$$
$$=\sum_j|\chi_j\rangle\langle\hat{\chi}_j|. \tag{D18}$$

These permit us to define a "natural" set of basis vectors,

$$|\hat{\alpha}\rangle\equiv G^{1/2}|\alpha\rangle=G^{-1/2}|\bar{\alpha}\rangle. \tag{D19}$$

We see immediately that

$$\langle\hat{\alpha}|\hat{\beta}\rangle=\langle\bar{\alpha}|G^{-1/2}G^{1/2}|\beta\rangle=\delta_{\alpha\beta}, \tag{D20}$$

showing that this natural basis is orthonormal. The new basis is, in a sense, just "halfway" between the $|\alpha\rangle$ and $|\bar{\alpha}\rangle$ bases. Even if there exist accidental degeneracies among the S_j's, the $|\hat{\alpha}\rangle$'s will be uniquely defined by the original $|\alpha\rangle$ basis. The "natural transformation" matrices are conveniently expressed as

$$G^{1/2}=\sum_{\alpha}|\hat{\alpha}\rangle\langle\bar{\alpha}|=\sum_{\alpha}|\bar{\alpha}\rangle\langle\hat{\alpha}|, \tag{D21}$$

$$G^{-1/2}=\sum_{\alpha}|\hat{\alpha}\rangle\langle\alpha|=\sum_{\alpha}|\alpha\rangle\langle\hat{\alpha}|. \tag{D22}$$

These relations are easy to illustrate in two dimensions. Figure 3 shows a nonorthogonal basis $|\alpha\rangle$, $|\beta\rangle$, and the corresponding $|\bar{\alpha}\rangle$ and $|\hat{\alpha}\rangle$ bases, as well as the "stretching axes" $|\hat{\chi}_1\rangle$, $|\hat{\chi}_2\rangle$. In this example, $S_1<1$, $S_2>1$. It is clear from (D20) that the norms of the $|\hat{\alpha}\rangle$'s are independent of the choice of norms n_α of the $|\alpha\rangle$ vectors. Not so obvious, perhaps, is the fact that the *directions* of the $|\hat{\alpha}\rangle$'s do depend on these norms. This is illustrated in Fig. 4.

Applications

In Sec. VII we obtained the linked-cluster expansion of a non-Hermitian matrix $\mathcal{W}_\infty$. This has real eigen-

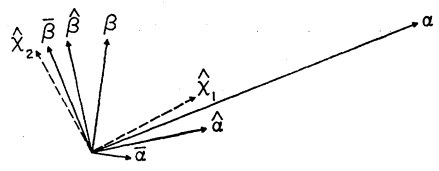


FIG. 4. Similar to Fig. 3, illustrating fact that the directions of the $|\alpha\rangle$'s depend on the norms of the $|\alpha\rangle$ vectors.

values, but its eigenvectors are generally not orthogonal:

$$\mathfrak{W}_\infty \mathbf{A}_\alpha = \Delta E_{V\alpha} \mathbf{A}_\alpha. \tag{D23}$$

(Apart from the core interaction energy ΔE_C, $\mathfrak{W}_\infty$ is equivalent to the $\mathfrak{A}$ operator of Bloch[54] and the h operator of Des Cloizeaux.[55]) The Hermitian conjugate matrix $\mathfrak{W}_\infty^\dagger$ defines a second set of eigenvectors:

$$\mathfrak{W}_\infty^\dagger \bar{\mathbf{A}}_\alpha = \Delta E_{V\alpha} \bar{\mathbf{A}}_\alpha. \tag{D24}$$

Combining this with (D23) gives

$$(\Delta E_{V\beta} - \Delta E_{V\alpha}) \bar{\mathbf{A}}_\beta^\dagger \mathbf{A}_\alpha = 0, \tag{D25}$$

which shows that the $\mathbf{A}_\alpha$'s and $\bar{\mathbf{A}}_\alpha$'s can be normalized to form a bi-orthogonal system. Assuming such a normalization, we find that

$$\mathfrak{W}_\infty = \sum_\alpha \mathbf{A}_\alpha \Delta E_{V\alpha} \bar{\mathbf{A}}_\alpha^\dagger = \sum_\alpha |\, \alpha \rangle \Delta E_{V\alpha} \langle \bar{\alpha} \,| \tag{D26}$$

$$\mathfrak{W}_\infty^\dagger = \sum_\alpha \bar{\mathbf{A}}_\alpha \Delta E_{V\alpha} \mathbf{A}_\alpha^\dagger = \sum_\alpha |\, \bar{\alpha} \rangle \Delta E_{V\alpha} \langle \alpha \,|. \tag{D27}$$

These representations are valid for any choice of the $\mathbf{A}_\alpha$ norms, provided the $\bar{\mathbf{A}}_\alpha$ norms are adjusted to satisfy (D3). (The corresponding natural basis vectors $\hat{\mathbf{A}}_\alpha$, however, *do* depend on the $\mathbf{A}_\alpha$ norms.) This freedom will enable us to find a simple expression for the natural transformation matrix $G^{1/2}$.

Consider the relations

$$\langle \Psi_\beta \,|\, \Psi_\alpha \rangle_V = \mathbf{A}_\beta^\dagger (\mathbf{I}+\Theta) \mathbf{A}_\alpha = \delta_{\alpha\beta} N_{V\alpha}, \tag{D28}$$

where we assume from now on that $\mathbf{A}_\alpha^\dagger \mathbf{A}_\alpha = 1$. These relations are equivalent to the matrix equation

$$\mathbf{I}+\Theta = \sum_\alpha \bar{\mathbf{A}}_\alpha N_{V\alpha} \bar{\mathbf{A}}_\alpha^\dagger. \tag{D29}$$

In abstract notation,

$$\mathbf{I}+\Theta = \sum_\alpha |\, \bar{\alpha} \rangle \langle \alpha \,|\, (\mathbf{I}+\Theta) \,|\, \alpha \rangle \langle \bar{\alpha} \,|, \tag{D30}$$

it is clear that this representation is invariant under the basis renormalization

$$\begin{aligned} |\, \alpha \rangle &\longrightarrow |\, \alpha' \rangle = C_\alpha \,|\, \alpha \rangle, \\ |\, \bar{\alpha} \rangle &\longrightarrow |\, \bar{\alpha}' \rangle = C_\alpha^{-1} \,|\, \bar{\alpha} \rangle. \end{aligned} \tag{D31}$$

By choosing $C_\alpha = (N_{V\alpha})^{-1/2}$, we obtain the desired simple results:

$$\mathbf{I}+\Theta = \sum_\alpha |\, \bar{\alpha}' \rangle \langle \bar{\alpha}' \,| = G, \tag{D32}$$

and

$$\begin{aligned} \hat{\mathbf{A}}_\alpha = G^{1/2} \mathbf{A}_\alpha' &= (\mathbf{I}+\Theta)^{1/2} \mathbf{A}_\alpha (N_{V\alpha})^{-1/2} \\ &= (\mathbf{I}+\Theta)^{1/2} \mathbf{A}_\alpha [\mathbf{A}_\alpha^\dagger (\mathbf{I}+\Theta) \mathbf{A}_\alpha]^{-1/2}. \end{aligned} \tag{D33}$$

The value of this "natural" basis becomes quite evident when we consider expectation values and transition amplitudes. Here we find a very simple result,

$$\begin{aligned} \langle \alpha \,|\, \mathcal{O} \,|\, \beta \rangle_V &\equiv \langle \Psi_\alpha \,|\, \mathcal{O} \,|\, \Psi_\beta \rangle_V / (N_{V\alpha} N_{V\beta})^{1/2} \\ &= (N_{V\alpha})^{-1/2} \mathbf{A}_\alpha^\dagger \odot \mathbf{A}_\beta (N_{V\beta})^{-1/2} \\ &= \hat{\mathbf{A}}_\alpha^\dagger (\mathbf{I}+\Theta)^{-1/2} \odot (\mathbf{I}+\Theta)^{-1/2} \hat{\mathbf{A}}_\beta. \end{aligned} \tag{D34}$$

The transition matrix $\mathfrak{M}$ is indeed given by (7.41), provided we use the natural basis vectors $\hat{\mathbf{A}}_\alpha$, $\hat{\mathbf{A}}_\beta$ instead of $\mathbf{A}_\alpha$, $\mathbf{A}_\beta$. We have already seen that (7.41) defines a linked-cluster expansion.

Des Cloizeaux has pointed out that the $\hat{\mathbf{A}}_\alpha$'s can be calculated as the eigenvectors of a *new* effective interaction matrix

$$\begin{aligned} \mathcal{K}_V &= G^{1/2} \mathfrak{W}_\infty G^{-1/2} \\ &= (\mathbf{I}+\Theta)^{1/2} \mathfrak{W}_\infty (\mathbf{I}+\Theta)^{-1/2} \\ &= \sum_\alpha \hat{\mathbf{A}}_\alpha \Delta E_{V\alpha} \hat{\mathbf{A}}_\alpha^\dagger. \end{aligned} \tag{D35}$$

The last of these relations follows from (D21), (D22), and (D26), and shows that $\mathcal{K}_V$ is indeed Hermitian. The second of these demonstrates that $\mathcal{K}_V$ and $\mathfrak{W}_\infty$ are nearly identical when Θ is nearly diagonal in some $\mathbf{A}_\beta^{(\alpha)}$ representation, or in other words when the $\mathbf{A}_\alpha$'s are nearly orthogonal. (The equivalence of these conditions should be obvious from Figs. 3 and 4.)

A linked-cluster expansion is obtained by methods analogous to (7.41), thus

$$\mathcal{K}_V = \sum_{r,s=0}^{\infty} \binom{\frac{1}{2}}{r} \binom{-\frac{1}{2}}{s} \Theta^r \mathfrak{W}_\infty \Theta^s, \tag{D36}$$

where the $(1+x)^{1/2}$ coefficients are

$$\binom{\frac{1}{2}}{r} = (r!)^{-1} \prod_{i=0}^{r-1} (\tfrac{1}{2} - i). \tag{D37}$$

The linked-cluster property is shown by the argument following (7.43), with one modification. For each value of t, the total weight of all different Θ-orderings with $r+s=t$ is now zero instead of unity. [Note that $\mathfrak{W}_\infty$ already consists of a single linked piece. There will also be some "extra terms," analogous to (7.21), which provide the desired corrections to $\mathfrak{W}_\infty$.]

The Hermiticity of $\mathcal{K}_V$ implies that its set of diagrams should be topologically invariant under reflection about a horizontal axis. In low orders, this can be checked term-by-term. This is *not* true for the diagrams of $\mathfrak{W}_\infty$. The expansion (D36) for $\mathcal{K}_V$ corresponds to a step-by-step symmetrization of $\mathfrak{W}_\infty$; a very reasonable procedure if the nonorthogonality of the *complete* set of $\mathbf{A}_\alpha$'s is weak. Furthermore, the rules for this

expansion are quite clear (although not simple), and one sees that a number of partial-summation techniques can still be used to advantage. On the other hand, there is much cancellation among the higher-order terms in (D36), and the general structure of the terms which remain is not at all clear. It is certainly not evident that the resulting set of diagrams is symmetric about a horizontal axis, as required by Hermiticity. A more concise characterization of the $\mathcal{K}_V$ diagrams would be helpful.

Some progress in this direction has been made by Des Cloizeaux, by way of a more compact notation. Since the $\mathcal{K}_V$ diagrams are symmetric while the time-ordering structure [see (7.14)] of the $\mathcal{W}_\infty$ diagrams is not, we apply the factorization theorem to the terms remaining after the elimination of unlinked parts. Following Des Cloizeaux, we introduce brackets as follows:

$$\{r_1, r_2, r_3, \cdots, r_n\}_L \equiv v_V(r_1)(-v_V(r_2))(-v_V(r_3))\cdots(-v_V(r_n))_L, \quad \text{(D38)}$$

where the $v_V(r)$'s are the same as in (7.2). The subscripts L are reminders that only the linked diagrams need be considered. The expansions can now be written quite compactly in terms of these brackets. To third order in v_V, they are

$$\mathcal{W}_\infty = \{0\}_L + \{1,0\}_L + \{2,0,0\}_L + \{1,1,0\}_L + \cdots, \quad \text{(D39)}$$

$$\Theta = \{1\}_L + \{2,0\}_L + \{0,2\}_L + \{0,1,2\}_L + \{2,1,0\}_L + \{3,0,0\}_L + \{0,3,0\}_L + \{0,0,3\}_L + \cdots, \quad \text{(D40)}$$

$$\mathcal{K}_V = \{0\} + \tfrac{1}{2}\{1,0\}_L + \tfrac{1}{2}\{0,1\}_L + \tfrac{3}{8}\{1,1,0\}_L + \tfrac{3}{8}\{0,1,1\}_L + \tfrac{1}{4}\{1,0,1\}_L + \tfrac{1}{2}\{2,0,0\}_L + \tfrac{1}{2}\{0,0,2\}_L + \cdots. \quad \text{(D41)}$$

Unfortunately, the general structure of this expansion for $\mathcal{K}_V$ is still not evident. The forms (D35), (D36) seem more practical and more transparent, even though they are not manifestly Hermitian. This defect is easily remedied by writing

$$\mathcal{K}_V = \tfrac{1}{2}[(1+\Theta)^{1/2}\mathcal{W}_\infty(1+\Theta)^{-1/2} + \text{h.c.}]. \quad \text{(D42)}$$

In this form, results will be Hermitian for approximations to any order in Θ.

This discussion of $\mathcal{K}_V$ is correct only for the case of exact degeneracy. For quasi-degenerate cases one would still like to have a secular equation of the form

$$[H_{0V} + \mathcal{K}_V]\hat{\mathbf{A}}_\alpha = 0. \quad \text{(D43)}$$

This requires the addition of an extra term,

$$(1+\Theta)^{1/2}H_{0V}(1+\Theta)^{-1/2} - H_{0V} = [(1+\Theta)^{1/2}, H_{0V}](1+\Theta)^{-1/2}, \quad \text{(D44)}$$

to the *unsymmetrized* expression (D35). This correction follows from (5.17). The *total* $\mathcal{K}_V$ may then be symmetrized, as in (D42). Upon expanding, the symmetrized correction is found to be

$$\tfrac{1}{8}\Theta^2 H_{0V} - \tfrac{1}{4}\Theta H_{0V}\Theta + \tfrac{1}{8}H_{0V}\Theta^2 + \mathcal{O}(\Theta^3). \quad \text{(D45)}$$

This should often be negligible, since it vanishes to first order in Θ.

Hermiticity of the Shell-Model Potential

The theory of the shell-model potential, as presented in Sec. 9 and Ref. 9, is not completely Hermitian. The eigenvalues are all real, but the one-body orbitals are not all mutually orthogonal. Formally, this problem is quite similar to the one just discussed. It can be solved in a similar way, by exploiting the correspondence $v_V(E_{V\alpha}) \leftrightarrow M^{\text{on}}(E_i)$ and $\Theta \leftrightarrow (-M'^{\text{on}})$. An interesting difference is that the "natural basis" $\hat{\phi}_i$ is now the one which has the most "physical" significance, in contrast to the nonorthogonal $\mathbf{A}_\alpha$ basis which represented projections of the complete wave functions. As a practical matter it may be easier to calculate the nonorthogonal ϕ_i basis, so we are now interested in *reversing* the sense of the transformation. The kinetic energy operator is far from being "degenerate," in the sense used above, and one will obtain a correction like (D44). Unfortunately, this will mar the simplicity of the "nonorthogonal" equations for the ϕ_m's. A number of the details deserve a careful discussion, and we shall reserve this for a future paper. We hope of course that the corrections are very weak. This problem deserves attention mainly for its intrinsic interest.

We should mention that a problem of this type was solved previously by Balian and DeDominicis.[119] They gave a prescription for their mass operator which is manifestly Hermitian. This appears to be closely related to the expansion (D41). That form is not convenient for reaction-matrix calculations, which is why we prefer the present approach.