Pseudo-Hamiltonian approach to a theory of effective interactions in the particle-hole channel: Microscopic foundations

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In an accompanying paper, we have described a new approach to the computation of ground-state energies and of correlated particle-hole excitations in terms of a phenomenological pseudo-Hamiltonian containing two- and more-body smooth effective potentials which sum the results of short-range correlations and of density fluctuation amplitudes which describe long-range correlations. In this paper we study the problem of relating the pseudopotentials to a (possibly singular) microscopic interaction with the aid of tools developed within the framework of the coupled cluster theory of Kümmel and his collaborators, the results containing both familiar and unfamiliar elements. For example, the formulas derived, which depend on Bethe-Goldstone and Bethe-Faddeev amplitudes, include new definitions of particle-hole scattering matrix elements. An important consistency check is satisfied, in that the problem of defining the phenomenological potentials in terms of the microscopic ones must yield two separate but equivalent solutions, once within the framework of the theory of the ground-state energy and a second time within the framework of the theory of excitations. The entire package is studied with the aid of a modified version of coupled cluster theory, and shown to form a self-consistent entity. Among the desirable features of the formalism is that the large gap in the single-particle energy spectrum often utilized in existing formalisms is naturally absent from the current one.

I. INTRODUCTION

The purpose of this paper is to supply the microscopic foundations for the phenomenological theory of binding energies and correlated particle-hole excitations described in an accompanying paper (referred to as I). In the latter we replace the "fundamental" many-particle (nonrelativistic) Hamiltonian,

$$H = t_{ab}\psi_a^\dagger\psi_b + \tfrac{1}{4}V_{abcd}\psi_a^\dagger\psi_b^\dagger\psi_d\psi_c \equiv \hat{K} + \hat{V} , \tag{1.1}$$

where we refer to I for notation, by a pseudo-Hamiltonian,

$$\overline{H} = \hat{K} + \hat{\overline{V}} , \tag{1.2}$$

where $\hat{\overline{V}}$, given in Eq. (2.2) of I, is a pseudointeraction consisting of a sum of two-, three-, . . . body smooth potentials. The basic strategy is superficially elementary in that we write (dropping the carets)

$$V = \overline{V} + (V - \overline{V}) \equiv \overline{V} + \tilde{V} , \tag{1.3}$$

where the last term may be called the fluctuation interaction. We demand that V be replaceable by $\overline{V}$, the pseudointeraction, for the purpose of describing the ground-state energy and particle-hole interactions. In other words, we require that the fluctuation interaction contribute nothing to the value of these observables.

What is possibly nontrivial is the process of transforming this elementary idea into a self-consistent theory. For this purpose, we have chosen some tools from coupled cluster theory[1] (CCT) and shown how these provide the necessary connections. Assuming a microscopic two-body interaction which contains a singular short-range repulsion, we demonstrate in Sec. II how the requirement that the microscopic and phenomenological Hamiltonians yield the same ground-state energy can be manipulated to provide definitions of the effective interactions. In this development, the structure of CCT introduces a distinction among different sets of matrix elements of the potential with respect to the chosen single-particle basis, which generalizes the familiar distinction between hole and particle single-particle energies. Thus, certain matrix elements of the interaction, including those necessary to calculate hole energies, are already well-defined by the two-particle Bethe-Goldstone (BG) function, whereas the particle-hole scattering elements necessary to define the particle energies involve the three-particle BG function even in lowest approximation. The definitions discovered involve in an essential way generalized BG wave functions.

In paper I we have insisted on using the same pseudo-Hamiltonian not only for the ground-state energy, but also for the construction of an extended random-phase approximation (RPA). We are faced thereby with a potentially severe consistency problem, in that this poses an additional set of requirements on the pseudo-Hamiltonian, a quantity that we had managed to define fully within the framework of the theory of the ground state. It is the burden of Sec. III to resolve this issue. We out-

line a demonstration that the independent definition of the smooth interaction from the standpoint of the equations of motion is equivalent to the definition found in the previous section.

In Sec. IV we turn to the problem of evaluating the effective potentials according to the definitions previously established. After a brief review and reformulation of the variational basis for CCT in its customary form, we show that the summation of the effects of microscopic interactions into effective potentials can lead to modified equations for the coupled cluster amplitudes and suggests a new method of solution in powers of the effective interaction. After further study, we see that one very desirable outcome (see below) is that particle as well as hole energies include potentials and that the gap in the single-particle spectrum which is natural to the usual form of CCT is effectively removed (Sec. V). We also regain in Sec. V the relation of the two-body effective potentials to the Brueckner K matrix, albeit in modified form.

Thus we end up with a reasonably coherent theoretical structure satisfying our aims to the order to which the theory is developed. Higher-order effects of potential interest will be described in subsequent publications.

Because we claim a new rearrangement of coupled cluster theory which fully includes long-range correlations, it is appropriate to comment on related CCT work. Thus Bishop and Lührmann[2] have shown how to deal exclusively with long-range correlations within the framework of CCT, but their elegant work assumes smooth microscopic potentials and is therefore not applicable to nuclear systems. The most elaborate coupled cluster calculations of Day,[3,4] which includes some ring diagrams, do not, apparently, include them fully. This has been discussed by Jackson,[5] who has argued that these calculations predict homogeneous nuclear matter in regimes of negative compressibility. The hypernetted chain variational calculations reported by Pandharipande and Wiringa[6] are subject to the same criticism. The theory discussed in our paper, since it contains the RPA computed with self-consistent effective forces, should exhibit the appropriate singular behavior in regions of negative compressibility.

One feature of our work to which we draw special attention is that we have made no use of model spaces in the sense of Ma and Kuo,[7] who have used this device to remove the energy gap at the Fermi surface and utilized it as part of a study of higher-order corrections[8] to Brueckner theory. The desirability of removing the energy gap in the single-particle spectrum has been advanced by Brown and collaborators[9,10] precisely in connection with their study of effective interactions within the framework of Landau theory and by Mahaux and his colleagues in their study of nuclear matter and of the optical potential.[11,12]

II. RELATION OF EFFECTIVE HAMILTONIAN TO MICROSCOPIC HAMILTONIAN BY MEANS OF COUPLED CLUSTER THEORY

In the preceding paper we have described a phenomenological theory of ground state energies and particle-hole excitations based upon a Hamiltonian containing a series of smooth effective interactions of two-body, three-body, . . . , type. In this paper, we shall show how these effective interactions can be related to the fundamental interaction which we allow to have a strong short-range repulsion or even a hard core. We calculate from (1.1)–(1.3),

$$\begin{aligned} W &= \langle G \mid H \mid G \rangle \\ &= \langle G \mid \bar{H} \mid G \rangle + \langle G \mid (\hat{V} - \hat{\bar{V}}) \mid G \rangle \\ &= \bar{W} + \langle G \mid (\hat{V} - \hat{\bar{V}} \mid G \rangle \ . \end{aligned} \tag{2.1}$$

We have previously evaluated $\bar{W}$. Since we want $W = \bar{W}$, our goal is evident: to relate the elements $\bar{V}_{abcd}$, $\bar{V}^{(2)}_{abcdef}, \ldots$ to the elements V_{abcd} so as to make the second term of (2.1) vanish. Remarkably this can be done provided we make use of a theorem from coupled cluster theory (CCT) and recognize the role played by many-body effective forces.

A. A decomposition theorem

We utilize a decomposition theorem due to Lührmann.[13] We shall write as in the CCT

$$\mid G \rangle = e^S \mid \phi \rangle / (\langle \phi \mid e^{S^\dagger} e^S \mid \phi \rangle)^{1/2} \ , \tag{2.2}$$

where $\mid \phi \rangle$ is the reference Slater determinant for the ground state, and S is the operator which describes the sum of linked clusters

$$\begin{aligned} S = \sum_{n=2} \frac{1}{(n!)^2} \psi^\dagger_{p_1} \cdots \psi^\dagger_{p_n} \psi_{h_n} \cdots \psi_{h_1} \\ \times S_n(p_1 \cdots p_n \mid h_1 \cdots h_n) \ , \end{aligned} \tag{2.3}$$

with $S_1(p \mid h) = 0$. (In the case of nuclear matter, $S_1 = 0$ is guaranteed by momentum conservation. The case of finite nuclei will be dealt with in future work.) The relations among the various amplitudes which occur in CCT and will be utilized below are summarized in Appendix A. We also introduce the unnormalized ground-state vector customarily employed in the CCT,

$$\mid \Psi \rangle = e^S \mid \phi \rangle \ . \tag{2.4}$$

Thus consider the matrix element

$$\begin{aligned} &\langle G \mid \psi^\dagger_a \psi^\dagger_b \psi_d \psi_c \mid G \rangle \\ &\qquad = \frac{\langle \phi \mid e^{S^\dagger} \psi^\dagger_a \psi^\dagger_b e^S I_{N-2} e^{-S} \psi_d \psi_c e^S \mid \phi \rangle}{\langle \phi \mid e^{S^\dagger} e^S \mid \phi \rangle} \ . \end{aligned} \tag{2.5}$$

Here I_{N-2} is the unit operator for the $(N-2)$ particle space, which may be written

$$\begin{aligned} I_{N-2} = \frac{1}{2!} \psi_{h_2} \psi_{h_1} \mid \phi \rangle \langle \phi \mid \psi^\dagger_{h_1} \psi^\dagger_{h_2} + \frac{1}{3!} \psi^\dagger_{p_1} \psi_{h_3} \psi_{h_2} \psi_{h_1} \mid \phi \rangle \\ \times \langle \phi \mid \psi^\dagger_{h_1} \psi^\dagger_{h_2} \psi^\dagger_{h_3} \psi_{p_1} + \cdots \ . \end{aligned} \tag{2.6}$$

By inserting (2.6) into (2.5), utilizing the definitions (2.2), (2.4), and the new definition (see below for discussion)

$$\begin{aligned} &\chi^{(12)}_n(a_1 a_2 p_3 \cdots p_n \mid h_1 \cdots h_n) \\ &\quad \equiv \langle \phi \mid \psi^\dagger_{h_1} \cdots \psi^\dagger_{h_n} \psi_{p_n} \cdots \psi_{p_3} e^{-S} \psi_{a_2} \psi_{a_1} \mid \Psi \rangle \ , \end{aligned} \tag{2.7}$$

we find the decomposition

$$\langle G \mid \psi_a^\dagger \psi_b^\dagger \psi_d \psi_c \mid G \rangle = \frac{1}{2!}\langle G \mid \psi_a^\dagger \psi_b^\dagger \psi_{h_2} \psi_{h_1} \mid G \rangle \chi_2^{(12)}(cd \mid h_1 h_2) + \frac{1}{3!}\langle G \mid \psi_a^\dagger \psi_b^\dagger \psi_{p_1}^\dagger \psi_{h_3} \psi_{h_2} \psi_{h_1} \mid G \rangle \chi_3^{(12)}(c\, dp_1 \mid h_1 h_2 h_3)$$
$$+ \frac{1}{4!}\frac{1}{2!}\langle G \mid \psi_a^\dagger \psi_b^\dagger \psi_{p_1}^\dagger \psi_{p_2}^\dagger \psi_{h_4} \cdots \psi_{h_1} \mid G \rangle \chi_4^{(12)}(c\, dp_1 p_2 \mid h_1 \cdots h_4) + \cdots . \tag{2.8}$$

The importance of this decomposition is the following: Suppose V actually contains a hard core. Let d and c in (2.8) be spatial coordinates (suppressing spin and isospin). Then because it is a physical amplitude, we demand that

$$\langle G \mid \psi_a^\dagger \psi_b^\dagger \psi(\mathbf{r}')\psi(\mathbf{r}) \mid G \rangle = 0, \quad |\mathbf{r}-\mathbf{r}'| < r_c , \tag{2.9}$$

where r_c is the hard-core radius. The quantities $\chi_n^{(12)}$ defined by (2.7) are generalized Bethe-Goldstone (Bethe-Faddeev) wave functions, each of which also possesses the property (2.9). Thus (2.8) is a decomposition in which each term preserves the property (2.9). We next describe how the decomposition theorem (2.8) provides a basis for the solution of the problem posed at the beginning of this section.

B. Conditions for determining the effective potentials

We are now prepared to study the conditions for the vanishing of the last term of (2.1). In this study the essential role of the multiparticle contributions to the effective forces will soon be apparent. From (2.1) and (2.8) and with $\tilde{V} = V - \bar{V}$ and $\bar{V} = \bar{V}^{(2)}$, the equations to determine the matrix elements of the effective forces are of the form

$$0 = \frac{1}{(2!)^2}\tilde{V}_{abcd}\left[\frac{1}{2!}\chi_2^{(12)}(cd \mid h_1 h_2)\langle G \mid \psi_a^\dagger \psi_b^\dagger \psi_{h_2}\psi_{h_1} \mid G \rangle + \frac{1}{3!}\chi_3^{(12)}(c\, dp_3 \mid h_1 h_2 h_3)\langle G \mid \psi_a^\dagger \psi_b^\dagger \psi_{p_3}^\dagger \psi_{h_3}\psi_{h_2}\psi_{h_1} \mid G \rangle\right.$$
$$\left. + \frac{1}{4!2!}\chi_4^{(12)}(c\, dp_3 p_4 \mid h_1 h_2 h_3 h_4)\langle G \mid \psi_a^\dagger \psi_b^\dagger \psi_{p_3}^\dagger \psi_{p_4}^\dagger \psi_{h_4}\psi_{h_3}\psi_{h_2}\psi_{h_1} \mid G \rangle + \cdots\right]$$
$$- \frac{1}{(3!)^2}\bar{V}^{(3)}_{abc,def}\left[\frac{1}{3!}\chi_3^{(123)}(de\, f \mid h_1 h_2 h_3)\langle G \mid \psi_a^\dagger \psi_b^\dagger \psi_c^\dagger \psi_{h_3}\psi_{h_2}\psi_{h_1} \mid G \rangle\right.$$
$$\left. + \frac{1}{4!}\chi_4^{(123)}(de\, fp_4 \mid h_1 h_2 h_3 h_4)\langle G \mid \psi_a^\dagger \psi_b^\dagger \psi_c^\dagger \psi_{p_4}^\dagger \psi_{h_4}\psi_{h_3}\psi_{h_2}\psi_{h_1} \mid G \rangle + \cdots\right]$$
$$- \frac{1}{(4!)^2}\bar{V}^{(4)}_{abcd,efgh}\left[\frac{1}{4!}\chi_4^{(1234)}(efgh \mid h_1 h_2 h_3 h_4)\langle G \mid \psi_a^\dagger \cdots \psi_d^\dagger \psi_{h_4}^\dagger \cdots \psi_{h_1} \mid G \rangle + \cdots\right] + \cdots . \tag{2.10}$$

We can verify that the matrix elements $\langle G \mid \psi_a^\dagger \cdots \psi_{h_1} \mid G \rangle$ are independent variables if the number of $\psi^\dagger$ and ψ therein are different and/or the suffixes on these operators are different. Therefore we obtain many equations by setting the coefficients of such independent variables in (2.10) equal to zero.

Before recording and studying these conditions, let us also note the basic assumptions by which we shall be enabled to understand their significance. (i) The terms $V\chi_n^{(12)}$ involving the microscopic two-body interaction must be kept together as a unit. (ii) The smooth effective interactions $\bar{V}$ may be treated perturbatively. (iii) The various orders may be identified by the use of decompositions of the χ_n defined in Appendix A, of which the simplest and most familiar is (A3), namely,

$$\chi_2^{(12)}(a_1 a_2 \mid h_1 h_2) = \delta(a_1 - h_1)\delta(a_2 - h_2) - \delta(a_2 - h_1)\delta(a_1 - h_2) + S_2(a_1 a_2 \mid h_1 h_2) . \tag{2.11}$$

It is then justified, when multiplied by $\bar{V}$ (as opposed to V) to treat S_2 as small compared to unity.

These assumptions are equivalent to the statements that S_{n+1} and $V\chi_{n+1}^{(12)}$ are of the order $(S_2)^n$ and that $\bar{V}^{(n+1)}$ is of order $(S_2)^n$ in lowest approximation. We shall make repeated use of these statements in the subsequent discussion.

As an illustration of this reasoning, from the coefficient of $\langle G \mid \psi_a^\dagger \psi_b^\dagger \psi_{h_2}\psi_{h_1} \mid G \rangle$ and (2.11) we obtain the condition

$$\bar{V}_{abh_1h_2} = \tfrac{1}{2}V_{abcd}\chi_2^{(2)}(cd \mid h_1 h_2) - \tfrac{1}{2}\bar{V}_{abp_1p_2}S_2(p_1 p_2 \mid h_1 h_2) . \tag{2.12}$$

According to our assumptions, the second term on the right-hand side of (2.12) is a correction term. Two remarks must be appended to this equation. First, it remains for us to specify a calculation procedure for the various amplitudes of CCT which appear here and will appear below. Since the phenomenology of the previous paper utilizes certain partial summations foreign to CCT, there will also be some modifications of the usual equations of this theory. These will be studied in Sec. IV. For the moment we assume only that these quantities are well defined and calculable. Second, as already emphasized, we are assuming in the rearrangement (2.12) that the second term on the right-hand side is a correction term. Here we seem to be somehow generating our special ver-

sion of a folded-diagram expansion.[14] Thus, in first approximation Eq. (2.12) determines the $\bar{V}_{abh_1h_2}$. For $(ab)=(ph)$, (hp), or (hh'), the correction terms will also be well specified, but for $(ab)=(pp')$ we require higher-order terms of the theory than considered in this paper.

Next, the coefficients of $\langle G \mid \psi_a^\dagger\psi_b^\dagger\psi_{p_3}^\dagger\psi_{h_3}\psi_{h_2}\psi_{h_1} \mid G\rangle$ and $\langle G \mid \psi_h^\dagger\psi_{h'}^\dagger\psi_{h''}^\dagger\psi_{h_3}\psi_{h_2}\psi_{h_1} \mid G\rangle$ yield the equations

$$\bar{V}_{abp_3,def}\chi_3^{(123)}(de\,f \mid h_1h_2h_3) = \tilde{V}_{abcd}\chi_3^{(12)}(c\,dp_3 \mid h_1h_2h_3)-(a\leftrightarrow p_3)-(b\leftrightarrow p_3)\,, \tag{2.13}$$

$$\bar{V}_{hh'h'',def}\chi_3^{(123)}(de\,f \mid h_1h_2h_3)=0\,. \tag{2.14}$$

According to our approximation scheme, to order $(S_2)^2$, (2.13) may be rewritten as

$$\bar{V}^{(3)}_{abp_3,h_1h_2h_3}=\tfrac{1}{6}[\tilde{V}_{abcd}\chi_3^{(12)}(c\,dp_3 \mid h_1h_2h_3)-(a\leftrightarrow p_3)-(b\leftrightarrow p_3)]-\tfrac{1}{2}\mathcal{A}(h_i)[\bar{V}^{(3)}_{abp_3,pp'h_3}S_2(pp' \mid h_1h_2)]\,, \tag{2.15}$$

where $\mathcal{A}(h_i)$ means the term as written minus $(h_3\leftrightarrow h_1)$ minus $(h_3\leftrightarrow h_2)$, i.e., it antisymmetrizes in the h_i between factors, where this is lacking.

We continue the analysis by considering the various choices for the pair (a,b) in (2.15). For $(a,b)=(h,h')$ the right-hand side of (2.15) contains the matrices $\bar{V}_{hh'cd}$ which are already given by (2.12), and thus (2.15) determines $\bar{V}^{(3)}_{hh'p,h_1h_2h_3}$ to order $(S_2)^2$, namely

$$\bar{V}_{hh'p_3,h_1h_2h_3}=\tfrac{1}{3}\{\tfrac{1}{2}V_{hh'cd}\chi_3^{(12)}(c\,dp \mid h_1h_2h_3)-\mathcal{A}(h_i)[\bar{V}_{hh'h_1p'}S_2(p'p \mid h_2h_3)]\}\,. \tag{2.16}$$

The derivation of (2.16) requires the application of (2.12) as well as the formulas of Appendix A.

For the case of $(a,b)=(h,p_2)$, the right-hand side of (2.15) contains $\bar{V}_{hp,h'p'}$, which is so far undefined even in order $(S_2)^1$. If we form a contraction by setting $h_3=h$ and summing over h, we obtain an equation which relates $\bar{V}_{hph'p}$ to $V\chi_3^{12}$ and $\bar{V}^{(3)}_{hp_2p_3,h_1h_2h}$. Since it is highly undesirable for the definition of $\bar{V}^{(n)}$ to depend on $\bar{V}^{(n+1)}$, this suggests that we impose the condition

$$\bar{V}^{(3)}_{hp_2p_3,h_1h_2h}=0\,. \tag{2.17}$$

In turn, this provides an equation to determine the so-far unknown $\bar{V}_{hph'p'}$, which is, in lowest order,

$$[\mathcal{A}(h_i)\bar{V}_{hp_2h_1p'}S_2(p'p_3 \mid h_2h_3)]_{h_3=h}=\tfrac{1}{2}V_{hp_2cd}\chi_3^{(12)}(c\,dp_3 \mid h_1h_2h)\,. \tag{2.18}$$

With $\bar{V}_{hph'p'}$, thus given [see Sec. V for an approximate evaluation of (2.18)], Eq. (2.15) defines $\bar{V}^{(3)}_{hpp',h_1h_2h_3}$. To the order $(S_2)^2$, we have

$$\bar{V}^{(3)}_{hp_2p_3,h_1h_2h_3}=\tfrac{1}{3}\mathcal{A}(p_i)\{\tfrac{1}{2}V_{hp_2cd}\chi_3^{(12)}(c\,dp_3 \mid h_1h_2h_3)-\mathcal{A}(h_i)[\bar{V}_{hp_2h_1p'}S_2(p'p_3 \mid h_2h_3)]\}\,. \tag{2.19}$$

For the remaining choice $(a,b)=(p_1,p_2)$, the previous strategem fails. Although the right-hand side of (2.15) contains the unknown $\bar{V}_{p_1p_2h'p'}$, we cannot form a contraction of $\bar{V}^{(3)}_{p_1p_2p_3,h_1h_2h_3}$ which is not trivially zero. Equation (2.15) will work as a definition of this latter three-body matrix element provided we can determine $\bar{V}_{p_1p_2p_3h'}$ in some independent manner (to be determined below).

Returning to (2.14), which has been ignored so far, it can be written to order $(S_2)^3$

$$\bar{V}^{(3)}_{hh'h'',h_1h_2h_3}=-\tfrac{1}{2}\mathcal{A}(h_i)[\bar{V}^{(3)}_{hh'h'',p_1p_2p_3}S_2(p_1p_2 \mid h_1h_2)]\,. \tag{2.20}$$

According to (2.19), (2.20) is well-defined and shows that the left-hand side vanishes to order $(S_2)^2$.

To complete our account, we return to (2.10) and consider the coefficient of $\langle G \mid \psi_a^\dagger\psi_b^\dagger\psi_{p_3}^\dagger\psi_{p_4}^\dagger\psi_{h_4}\psi_{h_3}\psi_{h_2}\psi_{h_1} \mid G\rangle$. We quote the consequent conditions only to the leading order $(S_2)^3$, namely

$$\bar{V}^{(4)}_{abp_3p_4,h_1\cdots h_4}=\tfrac{1}{12}[\tilde{V}_{abcd}\chi_4^{(12)}(c\,dp_3p_4 \mid h_1\cdots h_4)-(a\leftrightarrow p_3)-(a\leftrightarrow p_4)-(b\leftrightarrow p_3)-(b\leftrightarrow p_4)+(a\leftrightarrow p_3),(b\leftrightarrow p_4)]$$
$$-(\tfrac{1}{12})[\bar{V}^{(3)}_{abp_3,def}\chi_4^{(123)}(de\,fp_4 \mid h_1\cdots h_4)-(p_3\leftrightarrow p_4)-(a\leftrightarrow p_4)-(b\leftrightarrow p_4)]\,. \tag{2.21}$$

For the choice $(a,b)=(h,h')$ we encounter the undefined element $\bar{V}^{(3)}_{hh'p_3,h_1h_2p'}$, and therefore, in analogy to the above, setting $\bar{V}^{(4)}_{hh'p_3p_4,h_1h_2h_3h'}=0$, we eventually obtain the definition

$$\mathcal{A}(p_i)[\mathcal{A}(h_i)\bar{V}^{(3)}_{hh'p_3,h_1h_2p'}S_2(p'p_4 \mid h_3h_4)]_{h_4=h'}=\tfrac{1}{2}[\tilde{V}_{hh'cd}\chi_4^{(12)}(c\,dp_3p_4 \mid h_1h_3h_3h')]\,. \tag{2.22}$$

Similarly for $(a,b)=(h,p_2)$, by setting $\bar{V}^{(4)}_{hp_2p_3p_4,h_1h_2h_3h}=0$, we arrive at the equation

$$\mathcal{A}(p_i)[\mathcal{A}(h_i)\bar{V}^{(3)}_{hp_2p_3,h_1h_2p'}S_2(p'p_4 \mid h_3h_4)]_{h_4=h}=\tfrac{1}{2}\mathcal{A}(p_i)[\tilde{V}_{hp_2cd}\chi_4^{(12)}(c\,dp_3p_4 \mid h_1h_2h_3h)]\,, \tag{2.23}$$

which determines $\bar{V}^{(3)}_{hp_2p_3,h_1h_2p'}$.

The analysis of (2.23) is still incomplete. If we apply the formulas of Appendix A to $\chi_4^{(12)}$, we see that to order $(S_2)^2$, it has the form

$$\chi_4^{(12)}(c\,dp_3p_4\mid h_1\cdots h_4)\cong\mathcal{A}(h_i)[\delta_{ch_1}S_3(dp_3p_4\mid h_2h_3h_4)-(c\leftrightarrow d)]+\mathcal{A}(p_i\mid h_i)[S_2(cp_3\mid h_1h_3)S_2(dp_4\mid h_2h_4)]\ . \quad (2.24)$$

The terms $\sim(S_2)^2$ are multiplied by elements $\bar{V}_{hp_2pp'}$, so far undefined. This opportunity provides us with the missing definition of these elements. To see how this may be done in principle, we first replace (2.23) by the unsymmetrized version

$$\mathcal{A}(h_i)[\bar{V}^{(3)}_{hp_2p_3,h_1h_2p'}S_2(p'p_4\mid h_3h)]$$
$$=\tfrac{1}{2}\tilde{V}_{hp_4cd}\chi_4^{(12)}(c\,dp_2p_3\mid h_1h_2h_3h)\ , \quad (2.25)$$

that can be rewritten in the form

$$\sum_{h,p_3',h_1',h_2'}\bar{V}^{(3)}_{hp_2p_3,h_1'h_2'p'}A(hh_1'h_2'p',h_1h_2h_3p_4)$$
$$=\tfrac{1}{2}\sum_{h,c,d}\tilde{V}_{hp_4cd}\chi_4^{(12)}(c\,dp_2p_3\mid h_1h_2h_3h)\ , \quad (2.26)$$

where

$$A(hh_1'h_2'p',h_1h_2h_3p_4)=\delta_{h_1'h_1}\delta_{h_2'h_2}S_2(p'p_4\mid h_3h)$$
$$+\delta_{h_1'h_2}\delta_{h_2'h_3}S_2(p'p_4\mid h_1h)$$
$$+\delta_{h_1'h_3}\delta_{h_2'h_1}S_2(p'p_4\mid h_2h)\ . \quad (2.27)$$

Provided A has an inverse, we can solve (2.26),

$$\bar{V}^{(3)}_{hp_2p_3,h_1h_2p'}=\tfrac{1}{2}\tilde{V}_{h'p_4'cd}\chi_4^{(12)}(c\,dp_2p_3\mid h_1'h_2'h_3'h')$$
$$\times A^{-1}(h_1'h_2'h_3'p_4',hh_1h_2p')\ . \quad (2.28)$$

As the inverse matrix A^{-1} is not antisymmetric in the indices h and h_1 we can contract these indices in (2.28) and set the result $\bar{V}^{(3)}_{hp_2p_3,hh_2p'}=0$, thus providing the long-sought definition

$$\tilde{V}_{h'p_4'cd}\chi_4^{(12)}(c\,dp_2p_3\mid h_1'h_2'h_3'h')$$
$$\times A^{-1}(h_1'h_2'h_3'p_4',hhh_2p')=0\ . \quad (2.29)$$

In summary, we have by means of Eqs. (2.12), (2.18), and (2.29) provided the basis for computing the lowest approximation for the matrices $\bar{V}_{ab,h_1h_2}$, $\bar{V}_{php'h'}$, and $\bar{V}_{pp'p''h}$, namely, all elements of the two-body part of the effective interaction needed for the phenomenological theory of the preceding paper. We have also shown how the parts of $\bar{V}^{(3)}$ needed can also be obtained. It seems intuitively clear that the very natural approach of setting certain averages of many-body effective forces to zero as a way of determining lower-order pieces should generalize, though we shall not pursue this point further here. A more urgent task, postponed to Sec. V, is to explore the content of the formulas obtained thus far for $\bar{V}$.

III. DEFINITION OF EFFECTIVE INTERACTIONS WITHIN FRAMEWORK OF EXTENDED RPA CONSISTENCY WITH PREVIOUS DEFINITION

A. Equations of motion

In the preceding paper we have also described a phenomenological theory of particle-hole excitation, an extension of the RPA (RPA + damping) that was based on the pseudo-Hamiltonian. In this section we consider the means of deriving this model from the Hamiltonian (1.1) in which the interaction V may contain a repulsive core, even an infinite core. By writing again $V=\bar{V}+(V-\bar{V})\equiv\bar{V}+\tilde{V}$, we shall have as our goal to derive from the Hamiltonian (1.1) an equation of motion from which $\tilde{V}$, the short-range interaction is completely absent at least to the same order of accuracy to which the extended RPA was justified. This requirement must provide a set of definitions of the matrix elements of the effective potential. Furthermore, for consistency, these definitions must agree with those derived in Sec. II, as we have verified they do.

From the usual definitions

$$X_A(p\mid h)=\langle A\mid\psi_p^\dagger\psi_h\mid G\rangle\ , \quad (3.1)$$

$$Y_A(p\mid h)=\langle A\mid\psi_h^\dagger\psi_p\mid G\rangle\ , \quad (3.2)$$

we derive from the appropriate matrix elements of the commutators of $\psi_p^\dagger\psi_h$ and $\psi_h^\dagger\psi_p$ with H the following equations of motion:

$$-\omega_AX_A(p\mid h)=t_{hc}\langle A\mid\psi_p^\dagger\psi_c\mid G\rangle-\langle A\mid\psi_c^\dagger\psi_h\mid G\rangle t_{cp}$$
$$+\tfrac{1}{2}(\bar{V}_{hcde}+\tilde{V}_{hcde})\langle A\mid\psi_p^\dagger\psi_c^\dagger\psi_e\psi_d\mid G\rangle$$
$$-\tfrac{1}{2}(\bar{V}_{cdpe}+\tilde{V}_{cdpe})\langle A\mid\psi_c^\dagger\psi_d^\dagger\psi_e\psi_h\mid G\rangle\ , \quad (3.3)$$

$$-\omega_AY_A(p\mid h)=t_{pc}\langle A\mid\psi_h^\dagger\psi_c\mid G\rangle-\langle A\mid\psi_c^\dagger\psi_p\mid G\rangle t_{ch}$$
$$+\tfrac{1}{2}(\bar{V}_{pcde}+\tilde{V}_{pcde})\langle A\mid\psi_h^\dagger\psi_c^\dagger\psi_e\psi_d\mid G\rangle$$
$$-\tfrac{1}{2}(\bar{V}_{cdhe}+\tilde{V}_{cdhe})\langle A\mid\psi_c^\dagger\psi_d^\dagger\psi_e\psi_p\mid G\rangle\ , \quad (3.4)$$

where

$$\omega_A=W_A-W_G \quad (3.5)$$

is again the excitation energy of the state $\mid A\rangle$.

We assume that the terms involving t and $\bar{V}$ can be treated precisely as in the preceding paper and carried to the level of approximation which gives rise to the extended RPA. If the latter is understood to be a suitable phenomenology, then the task of this section consists of

finding the independent statements which will eliminate the contributions of $\tilde{V}$ to the required level of accuracy.

B. A decomposition theorem

In order to carry out our discussion we shall extend the decomposition theorem of Sec. II A. In addition to Eqs. (2.2)–(2.4) we introduce a representation for the state $|A\rangle$ in terms of an operator acting on the ground state,

$$|A\rangle = Q_A^\dagger |G\rangle \ . \tag{3.6}$$

Thus consider the matrix element

$$\langle A|\psi_a^\dagger\psi_b^\dagger\psi_d\psi_c|G\rangle = \langle\phi|e^{S^\dagger}Q_A\psi_a^\dagger\psi_b^\dagger e^S I_{N-2}e^{-S}\psi_d\psi_c e^S|\phi\rangle\langle\phi|e^{S^\dagger}e^S|\phi\rangle^{-1} \ . \tag{3.7}$$

Here I_{N-2} is the unit operator for the $(N-2)$ particle space, Eq. (2.6). By inserting this quantity into (3.7) and utilizing (2.2), (2.4), (2.6), and (3.6), we find, for instance

$$\begin{aligned}\langle A|\psi_a^\dagger\psi_b^\dagger\psi_d\psi_c|G\rangle = {}& \frac{1}{2!}\langle A|\psi_a^\dagger\psi_b^\dagger\psi_{h_2}\psi_{h_1}|G\rangle\chi_2^{(12)}(cd\,|\,h_1h_2) \\ & + \frac{1}{3!}\langle A|\psi_a^\dagger\psi_b^\dagger\psi_{p_1}^\dagger\psi_{h_3}\psi_{h_2}\psi_{h_1}|G\rangle\chi_3^{(12)}(c\,dp_1\,|\,h_1h_2h_3) \\ & + \frac{1}{4!}\langle A|\psi_a^\dagger\psi_b^\dagger\psi_{p_1}^\dagger\psi_{p_2}^\dagger\psi_{h_4}\cdots\psi_{h_1}|G\rangle\chi_4^{(12)}(c\,dp_1p_2\,|\,h_1\cdots h_4)+\cdots \ .\end{aligned} \tag{3.8}$$

This decomposition theorem is essential for the study of the term $\tilde{V}_{hcde}\langle A|\psi_p^\dagger\psi_c^\dagger\psi_e\psi_d|G\rangle$ of (3.3), where d and e take on all possible values. Thus in terms of special coordinates, $e\to\mathbf{r}'$, $d\to\mathbf{r}$ (suppressing spin and isospin), the matrix element

$$\langle A|\psi_p^\dagger\psi_c^\dagger\psi_{\mathbf{r}'}\psi_{\mathbf{r}}|G\rangle = 0, \quad |\mathbf{r}-\mathbf{r}'| < r_c \ , \tag{3.9}$$

when V has a hard core of radius r_c. Just as argued in Sec. II, each term of (3.8) maintains the hard-core property expressed by (3.9) because of the dependence on generalized Bethe-Goldstone wave functions. However, these observations are insufficient for the second relevant term of (3.3), namely $\tilde{V}_{cdpe}\langle A|\psi_c^\dagger\psi_d^\dagger\psi_e\psi_h|G\rangle$. In this case, in order to enforce the hard-core condition, we can derive an alternative to (3.8), in the form

$$\langle A|\psi_a^\dagger\psi_b^\dagger\psi_d\psi_c|G\rangle = \frac{1}{2!}\chi_{2A}^{(12)*}(ab\,|\,h_1h_2)\langle G|\psi_{h_1}^\dagger\psi_{h_2}^\dagger\psi_d\psi_c|G\rangle + \cdots \ , \tag{3.10}$$

where

$$\chi_{nA}^{(12)}(a_1a_2p_3\cdots p_n\,|\,h_1\cdots h_n) = \langle\phi|\psi_{h_1}^\dagger\cdots\psi_{h_n}^\dagger\psi_{p_n}\cdots\psi_{p_3}e^{-S}\psi_{a_2}\psi_{a_1}|A\rangle/\langle\phi|e^{S^\dagger}e^S|\phi\rangle]^{1/2} \tag{3.11}$$

are excited-state, generalized Bethe-Goldstone wave functions.[13] Though these functions have the same properties with respect to hard-core behavior as the set $\chi_n^{(12)}$, they are not useful to us in our present endeavor. Whereas we assume that the $\chi_n^{(12)}$ (at least for $n=2$, 3, and perhaps 4) are known from the CCT theory of the ground state, the calculation of the $\chi_{nA}^{(12)}$ requires an independent theory of the state $|A\rangle$, a theory that we are, in fact, trying to cast into the form of the extended RPA.

In order to circumvent this problem, utilizing (3.6), we write

$$\langle A|\psi_a^\dagger\psi_b^\dagger\psi_d\psi_c|G\rangle = \langle G|\psi_a^\dagger\psi_b^\dagger Q_A\psi_d\psi_c|G\rangle + \langle G|[Q_A,\psi_a^\dagger\psi_b^\dagger]\psi_d\psi_c|G\rangle \ . \tag{3.12}$$

In Appendix B we show that the second term of (3.19) is a kind of "blocking" correction to the first term of relative order $(1/N)$; it will, therefore, be neglected in what follows. It is also shown that we can apply Lührmann's decomposition to the first term, the result being

$$\begin{aligned}\langle G|\psi_a^\dagger\psi_b^\dagger Q_A\psi_d\psi_c|G\rangle = {}& \frac{1}{2!}\chi_2^{(12)*}(ab\,|\,h_1h_2)\langle A|\psi_{h_1}^\dagger\psi_{h_2}^\dagger\psi_d\psi_c|G\rangle \\ & + \frac{1}{3!}\chi_3^{(12)*}(abp_1\,|\,h_1h_2h_3)\langle A|\psi_{h_1}\psi_{h_2}^\dagger\psi_{h_3}^\dagger\psi_{p_1}\psi_d\psi_c|G\rangle \\ & + \frac{1}{4!}\frac{1}{2!}\chi_4^{(12)*}(abp_1p_2\,|\,h_1\cdots h_4)\langle A|\psi_{h_1}^\dagger\cdots\psi_{h_4}^\dagger\psi_{p_2}\psi_{p_1}\psi_d\psi_c|G\rangle + \cdots \ .\end{aligned} \tag{3.13}$$

This result should be compared with (3.8). The considerations which follow are based on the application of (3.8) and (3.13).

C. Definition of the effective potentials

We study the terms of Eqs. (3.3) and (3.4) which depend on $\tilde{V}$ in order to see to what extent we can make them vanish. In the course of doing so, we hope to thereby derive expressions for the matrix elements of $\bar{V}$. We shall include the

contributions of $\bar{V}^{(3)}$ explicitly in the formulas below, but not $\bar{V}^{(4)}$, though it should be remembered that the latter is also necessary to complete the program carried out in Sec. II. Thus with the help of (3.8) and (3.13) and their corresponding generalizations for the three-body Green's functions, we obtain from (3.3) the following two sets of conditions:

$$0\cong\tilde{V}_{hcde}\left[\frac{1}{2!}\chi_2^{(12)}(de\mid h_1h_2)\langle A\mid\psi_p^\dagger\psi_c^\dagger\psi_{h_2}\psi_{h_1}\mid G\rangle+\frac{1}{3!}\chi_3^{(12)}(de\,p_1\mid h_1h_2h_3)\langle A\mid\psi_p^\dagger\psi_c^\dagger\psi_{p_1}^\dagger\psi_{h_3}\psi_{h_2}\psi_{h_1}\mid G\rangle\right.$$
$$\left.+\frac{1}{4!}\frac{1}{2!}\chi_4^{(12)}(de\,p_1p_2\mid h_1\cdots h_4)\langle A\mid\psi_p^\dagger\psi_c^\dagger\psi_{p_1}^\dagger\psi_{p_2}^\dagger\psi_{h_4}\cdots\psi_{h_1}\mid G\rangle\right]$$
$$-\frac{1}{3!}\bar{V}^{(3)}_{hb_1b_2a_1a_2a_3}\left[\frac{1}{3!}\chi_3^{(123)}(a_1a_2a_3\mid h_1h_2h_3)\langle A\mid\psi_p^\dagger\psi_{b_1}^\dagger\psi_{b_2}^\dagger\psi_{h_3}\psi_{h_2}\psi_{h_1}\mid G\rangle\right.$$
$$\left.+\frac{1}{4!}\chi_4^{(123)}(a_1a_2a_3p_1\mid h_1\cdots h_4)\langle A\mid\psi_p^\dagger\psi_{b_1}^\dagger\psi_{b_2}^\dagger\psi_{p_1}^\dagger\psi_{h_4}\cdots\psi_{h_1}\mid G\rangle+\cdots\right], \tag{3.14}$$

$$0\cong\tilde{V}_{cdpe}\left[\frac{1}{2!}\chi_2^{(12)*}(cd\mid h_1h_2)\langle A\mid\psi_{h_1}^\dagger\psi_{h_2}^\dagger\psi_e\psi_h\mid G\rangle+\frac{1}{3!}\chi_3^{(12)*}(c\,dp_1\mid h_1h_2h_3)\langle A\mid\psi_{h_1}^\dagger\psi_{h_2}^\dagger\psi_{h_3}^\dagger\psi_{p_1}\psi_e\psi_h\mid G\rangle\right.$$
$$\left.+\frac{1}{4!}\frac{1}{2!}\chi_4^{(12)*}(c\,dp_1p_2\mid h_1\cdots h_4)\langle A\mid\psi_{h_1}^\dagger\cdots\psi_{h_4}^\dagger\psi_{p_2}\psi_{p_1}\psi_e\psi_h\mid G\rangle\right]$$
$$-\frac{1}{3!}\bar{V}^{(3)}_{a_1a_2a_3pb_1b_2}\left[\frac{1}{3!}\chi_3^{(123)*}(a_1a_2a_3\mid h_1h_2h_3)\langle A\mid\psi_{h_1}^\dagger\psi_{h_2}^\dagger\psi_{h_3}^\dagger\psi_{b_2}\psi_{b_1}\psi_h\mid G\rangle\right.$$
$$\left.+\frac{1}{4!}\chi_4^{(123)*}(a_1a_2a_3p_1\mid h_1\cdots h_4)\langle A\mid\psi_{h_1}^\dagger\cdots\psi_{h_4}^\dagger\psi_{p_1}\psi_{b_2}\psi_{b_1}\psi_h\mid G\rangle+\cdots\right], \tag{3.15}$$

where all the required χ functions are defined in Appendix A. We need not add the conditions which follow from (3.4), since up to complex conjugation they will be the same as those which follow from (3.14) and (3.15).

We shall not undertake a complete analysis, *ab initio,* of the context of Eqs. (3.14) and (3.15). All that is required is to show that this analysis can duplicate the results found in the preceding section. We shall only illustrate the basis for this desirable (and correct) conclusion. For instance, from the two-body Green's function terms of (3.14) and (3.15), we conclude that

$$\tilde{V}_{habc}\chi_2^{(12)}(bc\mid h_1h_2)=0\,, \tag{3.16}$$
$$\tilde{V}_{pabc}\chi_2^{(12)}(bc\mid h_1h_2)=0\,. \tag{3.17}$$

Together, we see that these equations duplicate (2.12) of Sec. II. The duplication of the remaining conditions of Sec. II requires some attention to questions of antisymmetry, but again occurs in pairs. We spare the reader the details.

We thus affirm the consistency of our theory to treat both the ground state and the low-lying excited states of a nucleus.

IV. VARIATIONAL PRINCIPLE FOR MODIFIED COUPLED CLUSTER THEORY

We have so far described a theory of ground-state binding which utilizes two sets of quantities, a set of effective interactions and a set of (extended) RPA amplitudes. The latter can be computed from equations of motion for fixed effective interactions, whereas the effective interactions have been shown to be determined from the microscopic Hamiltonian in terms of generalized Bethe-Faddeev amplitudes, as these are defined in CCT. A remaining task is therefore to explain how to calculate the latter.

We could, it appears, refer to a standard account and so bring this paper to an abrupt conclusion. We shall show, however, that this is not necessarily consistent with the rules of the game we have set up. In this game, the role of the effective interactions is to represent partial summations of the short-range correlations. Somehow the presence of these summations in a form not previously studied should be reflected in the equations which we utilize to compute the amplitudes that describe these correlations. To present this apparatus we shall employ a variational formulation of CCT due to Kümmel and Lührmann,[15] of which we have recently given an account.[16] In this section, in order to introduce the tools, we shall first give a concise derivation of the previous results and then show how they are modified by the requirements we have set. The basic tool is another decomposition theorem which combines the algebraic technique of the decomposition of Green's functions used in the previous section with certain well-known properties of their diagram expansions.

A. Another decomposition theorem

As an example, consider the two-particle Green's function

$$\langle G\mid\psi_p^\dagger\psi_{p'}^\dagger\psi_b\psi_a\mid G\rangle=\langle G\mid\psi_p^\dagger\psi_{p'}^\dagger I_{N-2}\psi_b\psi_a\mid G\rangle\,, \tag{4.1}$$

where I_{N-2} is the projection operator for the space of $(N-2)$ particles given in Eq. (2.6). We substitute the latter into (4.1) and utilize the definitions

$$F_n(p_1\cdots p_n \mid h_1\cdots h_n) = \langle \phi \mid \psi^\dagger_{h_1}\cdots\psi^\dagger_{h_n}\psi_{p_n}\cdots\psi_{p_1} \mid \Psi\rangle \ , \tag{4.2}$$

$$\psi_n(a_1a_2p_3\cdots p_n \mid h_1\cdots h_n) = \langle \phi \mid \psi^\dagger_{h_1}\cdots\psi^\dagger_{h_n}\psi_{p_n}\cdots\psi_{p_3}\psi_{a_2}\psi_{a_1} \mid \Psi\rangle \ , \tag{4.3}$$

where $\mid\Psi\rangle$ is the unnormalized ground-state vector, favored in CCT and related to $\mid G\rangle$ by the scale $\mathcal{F}_0$ [cf. (2.2) and (2.4)],

$$\mid G\rangle = \mathcal{F}_0 \mid \Psi\rangle \ , \tag{4.4}$$

$$\mathcal{F}_0^{-2} = \langle \phi \mid e^{S^\dagger}e^S \mid \phi\rangle \ . \tag{4.5}$$

The relations between S and the amplitudes (4.2) and (4.3) are summarized in Appendix A. They will be needed below. [We recall that both (4.2) and (4.3) describe "reducible" clusters which may contain unlinked parts and that (4.3) are subsystem wave functions[17] particularly useful in connection with hard-core interactions.]

The result of utilizing (2.6) and (4.3)–(4.5) in (4.1) allows the latter to be written

$$\langle G \mid \psi^\dagger_p\psi^\dagger_{p'}\psi_b\psi_a \mid G\rangle = \sum_{n=2}\frac{1}{n!(n-2)!}\mathcal{L}[\mathcal{F}_0^2F_n^*(pp'p_3\cdots p_n \mid h_1\cdots h_n)\psi_n(abp_3\cdots p_n)\mid h_1\cdots h_n)] \ , \tag{4.6}$$

where the symbol $\mathcal{L}$ means that only linked diagrams should be retained on the right-hand side of (4.6). Here we are making use of the property that diagram expansions of Green's functions contain only linked diagrams. By utilizing (4.4) and (4.5) we have "artificially" introduced unlinked pieces through the factors $\mathcal{F}_0$, and therefore we must remind the reader that all unlinked contributions will cancel. As argued in Ref. 16 a convenient way to rewrite the sum (4.6) is in the form

$$\langle G \mid \psi^\dagger_p\psi^\dagger_{p'}\psi_b\psi_a \mid G\rangle = \sum_{n=2}^{N}\frac{1}{n!(n-2)!}\Omega_n^*(pp'p_3\cdots p_n \mid h_1\cdots h_n)\psi_n(abp_3\cdots p_n \mid h_1\cdots h_n) \ . \tag{4.7}$$

Here Ω_n^* has no definition in terms of matrix elements (that we are aware of), but rather is a subset of diagrams which guarantees that the product $\Omega_n^*\psi_n$ consists only of the requisite linked diagrams. Thus Ω_n^* may be considered a subset of the diagrams of F_n^*, first recognized by Kümmel and Lührmann[15] as a natural set of variational quantities for the purposes at hand. We have $\Omega_0^*=1$ and for nuclear matter $\Omega_1^*=0$.

Other examples of results of the form (4.7) needed to evaluate (2.1) are

$$\langle G \mid \psi^\dagger_p\psi^\dagger_h\psi_b\psi_a \mid G\rangle = \sum_{n=1}\frac{(-1)}{n!(n-1)!}\Omega_n^*(pp_2\cdots p_n \mid h_1\cdots h_n)\psi_{n+1}(abp_2\cdots p_n \mid hh_1\cdots h_n) \ , \tag{4.8}$$

$$\langle G \mid \psi^\dagger_h\psi^\dagger_{h'}\psi_b\psi_a \mid G\rangle = \sum_{n=0}\frac{1}{(n!)^2}\Omega_n^*(p_1\cdots p_n \mid h_1\cdots h_n)\psi_{n+2}(abp_1\cdots p_n \mid hh'h_1\cdots h_n) \ , \tag{4.9}$$

$$\langle G \mid \psi_{h'}\psi^\dagger_h \mid G\rangle = \sum_{n=1}\frac{1}{n!(n-1)!}\Omega_n^*(p_1\cdots p_n \mid h_1\cdots h_{n-1}h')\psi_n(p_1\cdots p_n \mid h_1\cdots h_{n-1}h) \ , \tag{4.10}$$

$$\langle G \mid \psi^\dagger_p\psi_{p'} \mid G\rangle = \sum_{n=1}\frac{1}{n!(n-1)}\Omega_n^*(pp_2\cdots p_n \mid h_1\cdots h_n)\psi_n(p'p_2\cdots p_n \mid h_1\cdots h_n) \ . \tag{4.11}$$

B. Variational principle and equations of motion

We apply the previous decompositions to the ground-state expectation value of Eq. (2.1), written in the form

$$W = t_{hh} - \sum_h t_{hh}\langle G \mid \psi_h\psi^\dagger_h \mid G\rangle + \sum_p t_{pp}\langle G \mid \psi^\dagger_p\psi_p \mid G\rangle + \tfrac{1}{4}V_{pp'ab}\langle G \mid \psi^\dagger_p\psi^\dagger_{p'}\psi_b\psi_a \mid G\rangle$$
$$+\tfrac{1}{2}V_{phab}\langle G \mid \psi^\dagger_p\psi^\dagger_h\psi_b\psi_a \mid G\rangle + \tfrac{1}{4}V_{hh'ab}\langle G \mid \psi^\dagger_h\psi^\dagger_{h'}\psi_b\psi_a \mid G\rangle \ . \tag{4.12}$$

With the help of (4.7)–(4.11), we can write (4.12) as

$$W = t_{hh} + \tfrac{1}{4}V_{hh'ab}\psi_2(ab \mid hh')$$
$$+\sum_{n=2}\frac{1}{(n!)^2}\Omega_n^*(p_1\cdots p_n \mid h_1\cdots h_n)$$
$$\times[n(t_{p_1p_1}-t_{h_1h_1})\psi_n(p_1\cdots p_n \mid h_1\cdots h_n) + \tfrac{1}{4}n(n-1)V_{p_1p_2ab}\psi_n(abp_3\cdots p_n \mid h_1\cdots h_n)$$
$$-\tfrac{1}{2}nV_{p_1hab}\psi_{n+1}(abp_2\cdots p_n \mid hh_1\cdots h_n) + \tfrac{1}{4}V_{hh'ab}\psi_{n+2}(abp_1\cdots p_n \mid hh'h_1\cdots h_n)] \ . \tag{4.13}$$

By varying (4.13) with respect to Ω_n^* and taking due note of the necessity of antisymmetrizing the coefficient of $\delta\Omega_n^*$ in

the p_i and h_i indices, we obtain the equation of motion in its most concise form, suitable for use with a potential which has a hard core,[17] namely,

$$0=\mathcal{L}\mathcal{A}(p\mid h)[(t_{p_1p_1}-t_{h_1h_1})\psi_n(p_1\cdots p_n\mid h_1\cdots h_n)+\tfrac{1}{2}V_{p_1p_2ab}\psi_n(abp_3\cdots p_n\mid h_1\cdots h_n)$$

$$-\tfrac{1}{2}V_{p_1hab}\psi_{n+1}(abp_2\cdots p_n\mid hh_1\cdots h_n)+\tfrac{1}{4}V_{hh'ab}\psi_{n+2}(abp_1\cdots p_n\mid hh'h_1\cdots h_n)]\ , \tag{4.14}$$

where $\mathcal{A}$, as previously, is an antisymmetrization operator for each set of indices indicated, which requires exchanges only between two or more functions in an expression (not internally in ψ_n or V) and includes the usual factor of (-1) for each exchange. Equation (4.14) is transformed into an equation for the Bethe-Faddeev amplitudes $\chi_n^{(12)}$ by means of the equation

$$\psi_n(a_1a_2p_3\cdots p_n\mid h_1\cdots h_n)=\mathcal{A}(p\mid h)[\chi_n^{(12)}(a_1a_2p_3\cdots p_n\mid h_1\cdots h_n)$$

$$+\chi_{n-2}^{(12)}(a_1a_2p_3\cdots p_{n-2}\mid h_1\cdots h_{n-2})F_2(p_{n-1}p_n\mid h_{n-1}h_n)$$

$$+\cdots+\chi_2^{(12)}(a_1a_2\mid h_1h_2)F_{n-2}(p_3\cdots p_n\mid h_3\cdots h_n)]\ , \tag{4.15}$$

where, in a definition equivalent to (2.7),

$$\chi_n^{(12)}(a_1a_2p_3\cdots p_n\mid h_1\cdots h_n)=\langle\phi\mid\psi_{h_1}^\dagger\cdots\psi_{h_n}^\dagger\psi_{p_n}\cdots\psi_{p_3}e^{-S}\psi_{a_2}\psi_{a_1}e^S\mid\phi\rangle\ . \tag{4.16}$$

For further details, we refer to our previous work,[16] but more particularly to Refs. 1 and 17. Note, in particular, that in view of (4.14) the exact value of W is given by the first two terms of (4.13).

If we could solve Eqs. (4.14) exactly, we would, presumably, not need the auxiliary theory discussed below. The equations of this latter theory, insofar as our definitions of effective interactions are consistent, can only be a rearranged form of (4.14). The importance of this rearrangement, however, is that it suggests a new method of approximation.

For the new formulation we start with (2.1) and in accordance with our program drop the second term on the right-hand side since it is zero to the order of approximation to which we work. This can be verified directly, by using the decompositions (4.7)–(4.11) and the definitions of the effective interactions given in Sec. II. For this to work out we must include the elements $\bar{V}^{(3)},\ldots$. Similarly for the exact equivalence asserted these must then be included in W. An equivalent way of justifying that the second term of (2.1) can be omitted is to show, to the appropriate order, that the resulting equations of motion given by (4.25) below are equivalent to (4.14). For this again we have to include terms dependent on $\bar{V}^{(3)}$. However, for the sake of brevity, these terms are omitted in the remainder of this section.

Now the main new feature of $\bar{W}$ compared to the expression W treated in (4.12) is that the normal ordering has been carried out. Therefore in order to obtain a variational principle, we need some decompositions of the type (4.7)–(4.11) not given in the previous list. The additional expressions required can be obtained by examining Eqs. (2.6)–(2.11) of the accompanying paper, remembering that we have chosen to omit (2.12) from consideration. The following additional equations are derived by the same techniques used to derive (4.7)–(4.11):

$$\langle G\mid\psi_p^\dagger\psi_h\psi_{h'}^\dagger\psi_{p'}\mid G\rangle=\sum_{n=1}\frac{1}{(n!)^2}\Omega_{n+1}^*(pp_1\cdots p_n\mid hh_1\cdots h_n)\psi_{n+1}(p'p_1\cdots p_n\mid h'h_1\cdots h_n)\ , \tag{4.17}$$

$$\langle G\mid\psi_p^\dagger\psi_{p'}^\dagger\psi_h\psi_h\mid G\rangle=\sum_{n=2}\frac{1}{[(n-2)!]^2}\Omega_n^*(pp'p_1\cdots p_{n-2}\mid hh'h_1\cdots h_{n-2})\psi_{n-2}(p_1\cdots p_{n-2}\mid h_1\cdots h_{n-2})\ , \tag{4.18}$$

$$\langle G\mid\psi_h^\dagger\psi_{h'}^\dagger\psi_p\psi_p\mid G\rangle=\sum_{n=0}\frac{1}{(n!)^2}\Omega_n^*(p_1\cdots p_n\mid h_1\cdots h_n)\psi_{n+2}(pp'p_1\cdots p_n\mid hh'h_1\cdots h_n)\ , \tag{4.19}$$

$$\langle G\mid\psi_p^\dagger\psi_h\psi_{p'}^\dagger\psi_{p''}\mid G\rangle=\sum_{n=1}\frac{1}{n!}\frac{1}{(n-1)!}\Omega_{n+1}^*(pp'p_2\cdots p_n\mid hh_1\cdots h_n)\psi_n(p''p_2\cdots p_n\mid h_1\cdots h_n)\ , \tag{4.20}$$

$$\langle G\mid\psi_{p''}^\dagger\psi_{p'}\psi_h^\dagger\psi_p\mid G\rangle=\sum_{n=1}\frac{1}{n!}\frac{1}{(n-1)!}\Omega_n^*(p''p_2\cdots p_n\mid h_1\cdots h_n)\psi_{n+1}(pp'p_2\cdots p_n\mid hh_1\cdots h_n)\ , \tag{4.21}$$

$$\langle G\mid\psi_p^\dagger\psi_{h''}\psi_{h'}\psi_h^\dagger\mid G\rangle=\sum_{n=1}\frac{(-1)}{n!(n-1)!}\Omega_{n+1}^*(pp_1\cdots p_n\mid h'h''h_2\cdots h_n)\psi_n(p_1\cdots p_n\mid hh_2\cdots h_n)\ , \tag{4.22}$$

$$\langle G\mid\psi_h\psi_{h'}^\dagger\psi_{h''}^\dagger\psi_p\mid G\rangle=\sum_{n=1}\frac{(-1)}{n!(n-1)!}\Omega_n^*(p_1\cdots p_n\mid hh_2\cdots h_n)\psi_{n+1}(pp_1\cdots p_n\mid h'h''h_2\cdots h_n)\ . \tag{4.23}$$

For the expression which "replaces" (4.13) (but as written is only an approximation to it because of stated omissions) we have

$$\overline{W}=t_{hh}+\tfrac{1}{2}\overline{V}_{hh'hh'}+\tfrac{1}{4}\overline{V}_{hh'pp'}\psi_2(pp'\mid hh')$$
$$+\sum_{n=2}\frac{1}{(n!)^2}\Omega_n^*(p_1\cdots p_n\mid h_1\cdots h_n)$$
$$\times[n(\epsilon_{p_1}-\epsilon_{h_1})\psi_n(p_1\cdots p_n\mid h_1\cdots h_n)+n^2\overline{V}_{p_1hh_1p}\psi_n(pp_2\cdots p_n\mid hh_2\cdots h_n)$$
$$+\tfrac{1}{4}n^2(n-1)^2\overline{V}_{p_1p_2h_1h_2}\psi_{n-2}(p_3\cdots p_n\mid h_3\cdots h_n)+\tfrac{1}{4}\overline{V}_{hh'pp'}\psi_{n+2}(pp'p_1\cdots p_n\mid hh'h_1\cdots h_n)$$
$$+\tfrac{1}{2}n^2(n-1)\overline{V}_{p_1p_2h_1p}\psi_{n-1}(pp_3\cdots p_n\mid h_2\cdots h_n)+\tfrac{1}{2}n\overline{V}_{hp_1pp'}\psi_{n+1}(pp'p_2\cdots p_n\mid hh_1\cdots h_n)$$
$$-\tfrac{1}{2}n^2(n-1)\overline{V}_{p_1hh_1h_2}\psi_{n-1}(p_2\cdots p_n\mid hh_3\cdots h_n)-\tfrac{1}{2}n\overline{V}_{hh'ph_1}\psi_{n+1}(pp_1\cdots p_n\mid hh'h_2\cdots h_n)]\ . \tag{4.24}$$

The derivation of the equations of motion proceeds as in the transition from (4.13) to (4.14) and yields

$$0=\mathcal{L}\mathcal{A}(p\mid h)[(\epsilon_{p_1}-\epsilon_{h_1})\psi_n(p_1\cdots p_n\mid h_1\cdots h_n)+\overline{V}_{p_1hh_1p}\psi_n(pp_2\cdots p_n\mid hh_2\cdots h_n)$$
$$+\overline{V}_{p_1p_2h_1h_2}\psi_{n-2}(p_3\cdots p_n\mid h_3\cdots h_n)+\tfrac{1}{4}\overline{V}_{hh'pp'}\psi_{n+2}(pp'p_1\cdots p_n\mid hh'h_1\cdots h_n)$$
$$+\overline{V}_{p_1p_2h_1p}\psi_{n-1}(pp_3\cdots p_n\mid h_2\cdots h_n)+\tfrac{1}{2}\overline{V}_{hp_1pp'}\psi_{n+1}(pp'p_2\cdots p_n\mid hh_1\cdots h_n)$$
$$-\overline{V}_{p_1hh_1h_2}\psi_{n-1}(p_2\cdots p_n\mid hh_3\cdots h_n)-\tfrac{1}{2}\overline{V}_{hh'h_1p}\psi_{n+1}(pp_1\cdots p_n\mid hh'h_2\cdots h_n)]\ . \tag{4.25}$$

At this point there remains the exercise of proving that (4.25), with the addition of the terms depending on $\overline{V}^{(3)}$ and to the order of the accuracy of the definitions of $\overline{V}$ and $\overline{V}^{(3)}$ presented in Sec. II can be transformed back to (4.14). We have verified this result for $n=2$ and $n=3$ explicitly, but choose to spare the reader the details, which are somewhat lengthy, especially for $n=3$. The main point to emphasize once more is that (4.25) presents us with a new aspect of coupled cluster theory, suggesting, insofar as the effective potentials are smooth and sufficiently weak, that we can solve the equations by perturbation in powers of $\overline{V}$.

As the remaining task that we have set for ourselves in this paper, we consider below an approximate evaluation of the two-body effective potentials.

V. APPROXIMATE EVALUATION OF TWO-BODY EFFECTIVE POTENTIALS

A. Two-body equations

Let us start with the full form of (4.25) for $n=2$, rewritten (and rearranged) with the aid of (4.15), (A3), and (A4). We find

$$(\epsilon_{h_1}+\epsilon_{h_2}-\epsilon_{p_1}-\epsilon_{p_2})S_2(p_1p_2\mid h_1h_2)=\overline{V}_{p_1p_2h_1h_2}+\mathcal{A}(p\mid h)\overline{V}_{p_1hh_1p}S_2(pp_2\mid hh_2)$$
$$+\tfrac{1}{2}[\overline{V}_{hp_1pp'}S_3(pp'p_2\mid hh_1h_2)-(p_1\leftrightarrow p_2)]$$
$$-\tfrac{1}{2}[\overline{V}_{hh'ph_1}S_3(pp_1p_2\mid hh'h_2)-(h_1\leftrightarrow h_2)]$$
$$+\tfrac{1}{4}\mathcal{L}\{\overline{V}_{hh'pp'}[S_4(pp'p_1p_2\mid hh'h_1h_2)+\mathcal{A}(p\mid h)S_2(pp'\mid hh')S_2(p_1p_2\mid h_1h_2)]\}\ . \tag{5.1}$$

According to our elementary notions, we are to solve (5.1) as a series in $\overline{V}$. Since S_2 is then at least first order in $\overline{V}$, S_3 (as we shall see) second order, etc., the leading approximation is

$$(\epsilon_{h_1}+\epsilon_{h_2}-\epsilon_{p_1}-\epsilon_{p_2})S_2(p_1p_2\mid h_1h_2)\cong\overline{V}_{p_1p_2h_1h_2}=\tfrac{1}{2}V_{p_1p_2ab}\chi_2^{(12)}(ab\mid h_1h_2)-\tfrac{1}{2}\overline{V}_{p_1p_2p_1'p_2'}S_2(p_1'p_2'\mid h_1h_2)\ . \tag{5.2}$$

If we agree to ignore the last term of (5.2) since it is of the order of other terms of (5.1) which have been shelved, the resulting equation is of the familiar Bethe-Goldstone form, except that not only are the hole energies modified by a hole potential related to (2.17) but also the particle energies include a potential which is to be calculated according to the recipe given at the end of Sec. II involving three-particle contributions (and to be discussed further below). Thus we must consider, as we shall shortly, the three-body problem. Before proceeding, however, we shall use (5.2) to define what we shall mean by the Brueckner K matrix for the remainder of our discussion [that, except for the presence of the ϵ_p in (5.2) is the standard definition],

$$K_{abh_1h_2}(\epsilon_{h_1}+\epsilon_{h_2})\equiv\tfrac{1}{2}V_{abcd}\chi_2^{(12)}(cd\mid h_1h_2)\ . \tag{5.3}$$

If we define an off-shell version by the equation

$$K_{abh_1h_2}[E]=V_{abh_1h_2}+\tfrac{1}{2}\sum_{p_1p_2}V_{abp_1p_2}\frac{1}{E-\epsilon_{p_1}-\epsilon_{p_2}}K_{p_1p_2h_1h_2}[E]\ , \tag{5.4}$$

which is an equation for $(a,b)=(p,p')$ and a definition otherwise. The solution of (5.2) is provided through (5.3). Thus we see in lowest approximation an essentially familiar result, namely

$$\bar{V}_{abh_1h_2}=K_{abh_1h_2}(\epsilon_{h_1}+\epsilon_{h_2})\ . \tag{5.5}$$

From (5.2) we note furthermore that $S_2\sim\bar{V}$, which is the basis for past and subsequent reasoning.

Before continuing on to study three-body equations for other matrix elements of $\bar{V}$, it is necessary to comment that in just one sense our scheme is not strictly perturbative in $\bar{V}$. This proviso applies to the treatment of the single-particle potentials. Here it is natural to treat the complete single-particle energies as zero-order quantities. This point of view arose in a natural way from the structure of the phenomenological theory.

B. Three-body equations

Here, for orientation and for utilization below, we keep only the leading terms, namely

$$\epsilon(h_1h_2h_3\mid p_1p_2p_3)S_3(p_1p_2p_3\mid h_1h_2h_3)=\mathcal{A}(p\mid h)[\bar{V}_{p_1p_2h_1p}S_2(pp_3\mid h_2h_3)-\bar{V}_{p_1hh_1h_2}S_2(p_2p_3\mid hh_3)]\ , \tag{5.6}$$

where

$$e(h_1h_2h_3\mid p_1p_2p_3)\equiv\epsilon_{h_1}+\epsilon_{h_2}+\epsilon_{h_3}-\epsilon_{p_1}-\epsilon_{p_2}-\epsilon_{p_3}\ . \tag{5.6a}$$

In the second term of (5.6) we substitute (5.5). For the first term, we recognize the combination which occurs in (2.16). Together with the help of (A3) and (A4), we can now write (5.6) in the form

$$e(h_1h_2h_3\mid p_1p_2p_3)S_3(p_1p_2p_3\mid h_1h_2h_3)=\mathcal{A}(p\mid h)\bar{\bar{V}}(p_1p_2p_3\mid h_1h_2h_3)+\tfrac{1}{2}\mathcal{A}(p)V_{p_1p_2p'_1p'_2}S_3(p'_1p'_2p_3\mid h_1h_2h_3)\ , \tag{5.7}$$

where

$$\bar{\bar{V}}(p_1p_2p_3\mid h_1h_2h_3)=V_{p_1p_2h_1p}S_2(pp_3\mid h_2h_3)-S_2(p_1p_2\mid hh_1)K_{p_3hh_2h_3}(\epsilon_{h_2}+\epsilon_{h_3})-6\bar{V}^{(3)}_{p_1p_2p_3h_1h_2h_3}\ . \tag{5.8}$$

To simplify the discussion and reduce the result we are looking to a familiar form, we seize upon a distinction among the three terms of (5.8). For a strong short-range repulsion only the first term becomes singular [that singularity cancelling against the remaining term of (5.7) which arose from the decomposition of $\chi_S^{(12)}$]. For this reason and by power counting in S_2 it seems reasonable to retain initially only the first term of (5.8). Under these circumstances (5.7) becomes a version of the Bethe-Faddeev equations, modified only by the new energies. We review briefly the treatment of this equation by multiple scattering theory.

It is important for the sequel to notice that here and also below the partial antisymmetrizing operator $\mathcal{A}$ is equivalent to a sum over cyclic permutations of the indices involved. Conversion to a familiar form of multiple scattering theory occurs when we first introduce a three-body T matrix,

$$T_3(p_1p_2p_3\mid h_1h_2h_3)=\epsilon(h_1h_2h_3\mid p_1p_2p_3)S_3(p_1p_2p_3\mid h_1h_2h_3)\ , \tag{5.9}$$

and further decompose T_3,

$$T_3=T_3^{(3)}+T_3^{(2)}+T_3^{(1)}\ , \tag{5.10}$$

where, for example, $T_3^{(3)}$ is that part of T_3 where the last interaction is between particles 1 and 2 (and thus 3 is the spectator). This decomposition also expresses the sum over cyclic permutations, and therefore each $T_3^{(i)}$ is antisymmetric in a single pair of particle indices.

By means of (5.9) and (5.10) the simplified version of (5.7) becomes equivalent to the equation

$$T_3^{(3)}(p_1p_2p_3\mid h_1h_2h_3)=\mathcal{A}(h)[V_{p_1p_2h_1p'_2}S_2(p'_2p_3\mid h_2h_3)]+\tfrac{1}{2}V_{p_1p_2p'_1p'_2}\frac{1}{e(h_1h_2h_3\mid p'_1p'_2p_3)}T_3(p'_1p'_2p_3\mid h_1h_2h_3)\ , \tag{5.11}$$

plus the two equations obtained by cyclic permutation of p_1, p_2, and p_3. Equations (5.10) and (5.11) may be combined, and a further standard algebraic manipulation carried out in order to replace the elements of V by those of a suitable K matrix, as defined by (5.4). This yields, for example,

$$\begin{aligned}T_3^{(3)}(p_1p_2p_3\mid h_1h_2h_3)=&\,\mathcal{A}(h)K_{p_1p_2h_1p'_2}(\epsilon_{h_1}+\epsilon_{h_2}+\epsilon_{h_3}-\epsilon_{p_3})S_2(p'_2p_3\mid h_2h_3)\\&+\tfrac{1}{2}K_{p_1p_2p'_1p'_2}(\epsilon_{h_1}+\epsilon_{h_2}+\epsilon_{h_3}-\epsilon_{p_3})e(h_1h_2h_3\mid p'_1p'_2p_3)^{-1}\\&\times[T_3^{(2)}(p'_1p'_2p_3\mid h_1h_2h_3)+T_3^{(1)}(p'_1p'_2p_3\mid h_1h_2h_3)]\ ,\end{aligned} \tag{5.12}$$

and cyclic perturbations.

Before applying these (well-known) results to the "solution" of (2.18), one further remark is necessary for later use. Note that just as Eq. (4.3) is an equation to determine $K_{p_1p_2h_1h_2}(E)$, but that for any other matrix element $K_{abh_1h_2}(E)$, it is a definition of the latter, in the same way, we may extend Eqs. (5.11) to general elements $T_3^{(i)}(a_1a_2p \mid h_1h_2h_3)$, where a_i may be a particle or hole label.

We wish to apply these results on the three-body problem to Eqs. (2.18), which represents our definition of $\bar{V}_{php'h'}$. In order to do so, we must note that our approximation to the right-hand side of (5.7) may also be written

$$\mathcal{A}(p_i)V_{p_1p_2cd}\chi_3^{(12)}(c\,dp_3 \mid h_1h_2h_3)\ . \tag{5.13}$$

Comparison with (2.18) is highly suggestive and taking due note of (5.9) and sequel, we find that (2.18) is equivalent to the equation

$$[\mathcal{A}(h_i)\bar{V}_{hp_2h_1p'}S_2(p'p_3 \mid h_2h_3)]_{h_3=h} = T_3^{(3)}(hp_2p_3 \mid h_1h_2h)\ . \tag{5.14}$$

Though strictly against the rules of the hole line expansion, let us for orientational purposes replace the right-hand side of (5.14) by the first term of the right-hand side of (5.12), its Born approximation. We thus obtain

$$[\mathcal{A}(h_i)\bar{V}_{hp_2h_1p'}S_2(p'p_3 \mid h_2h_3)]_{h_3=h} \cong [\mathcal{A}(h_i)K_{hp_2h_1p'}(\epsilon_{h_1}+\epsilon_{h_2}+\epsilon_{h_3}-\epsilon_{p_3})S_2(p'p_3 \mid h_2h_3)]_{h_3=h}\ . \tag{5.15}$$

If the K matrix depends only weakly on its starting energy, this equation has the approximate solution

$$\bar{V}_{hph_1p_1} \cong K_{hph_1p_1}(\epsilon_{h_1}+\epsilon_{p_1})\ . \tag{5.16}$$

Even though a more accurate solution of (2.18) will differ quantitatively from (5.16), the main qualitative point which emerges from this consideration is that we expect our definitions to largely remove the gap in single-particle energies at the Fermi surface. It is easy to believe that a result similar to (5.16) can be extracted from (2.29) for the elements $\bar{V}_{hpp_1p_2}$, in further support of the above conclusion. We will spare the reader the somewhat more arduous details of this demonstration, however.

VI. CONCLUDING REMARKS

In this paper we have supplied the microscopic underpinnings of a new phenomenology for low-energy nuclear physics in the particle-hole channel. The theory utilizes in an essential way the tools of coupled cluster theory. We have purposely avoided the introduction of model spaces. Within CCT, we have produced what appear to be consistent definitions of the two-body effective forces. It also became clear why many-body effective forces are necessary, and we have shown how some of these may be calculated. A major result of our presentation is the proof that the same pseudo-Hamiltonian can be utilized for the ground-state energy as for the theory of low-energy excitations based on the RPA including damping.

Though we have presented sufficient grounds for optimism, it remains to be seen whether the formalism can be fully extended to higher order. But even to the order to which the theory has been developed in this paper, it appears to provide a natural foundation for Hartree-Fock theory and a systematic approach to the calculation of correction terms, in a form which can be carried out for finite nuclei.

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APPENDIX A: SUMMARY OF THE PROPERTIES OF THE GENERALIZED BETHE-GOLDSTONE FUNCTIONS

We study first the functions which occur in connection with two-particle interactions

$$\chi_n^{(12)}(a_1a_2p_3\cdots p_n \mid h_1\cdots h_n) = \langle \phi \mid \psi^\dagger\cdots\psi_{h_n}^\dagger\psi_{p_n}\cdots\psi_{p_3}e^{-S}\psi_{a_2}\psi_{a_1} \mid \Psi\rangle\ . \tag{A1}$$

Considering the separate possibilities for a_i, namely hole or particle label, using the anticommutation relations, the properties of $\mid\phi\rangle$ that it is annihilated by ψ_p or $\psi_h^\dagger$, the definitions (4.2) and (4.3) as well as the statement

$$[\psi_a, e^S] = e^S[\psi_a, S], \quad \{a\}=\{p\}\ , \tag{A2}$$

we easily find for $\chi_n^{(12)}$,

$$\chi_n^{(12)}(a_1a_2p_3\cdots p_n \mid h_1\cdots h_n)=\delta_{n,2}[\delta(a_1-h_1)\delta(a_2-h_2)-(a_1\leftrightarrow a_2)]$$
$$+\mathcal{A}(a \mid h)\delta(a_1-h_1)\langle\phi \mid \psi_{h_2}^\dagger\cdots\psi_{h_n}^\dagger\psi_{p_n}\cdots\psi_{p_3}[\psi_{a_2},S] \mid \phi\rangle$$
$$+\langle\phi \mid \psi_{h_1}^\dagger\cdots\psi_{h_n}^\dagger\cdots\psi_{p_3}\{[\psi_{a_2},[\psi_{a_1},S]]+[\psi_{a_2},S][\psi_{a_1},S]\} \mid \phi\rangle$$
$$=\delta_{n,2}[\delta(a_1-h_1)\delta(a_2-h_2)-(a_1\leftrightarrow a_2)]$$
$$+\mathcal{A}(a \mid h)\delta(a_1-h_1)S_{n-1}(a_2\cdots p_n \mid h_2\cdots h_n)$$
$$+F_n^{(12)}(a_1a_2p_3\cdots p_n \mid h_1\cdots h_n)\ , \tag{A3}$$

where

$$F_n^{(12)}(a_1a_2p_3\cdots p_n \mid h_1\cdots h_n)=S_n(a_1a_2p_3\cdots p_n \mid h_1\cdots h_n)+\sum_{n_1}\mathcal{A}(p \mid h)S_{n_1}(a_1p_3\cdots p_{n_1+1} \mid h_1\cdots h_{n_1})$$
$$\times S_{n-n_1}(a_2p_{n_1+2}\cdots p_n \mid h_{n_1+1}\cdots h_n)\ . \tag{A4}$$

In (A3) and (A4) the symbol $\mathcal{A}(a \mid b \mid c\cdots)$ means carry out all distinct permutations of each of sets $\{a\},\{b\},\{c\}\cdots$, which involve exchanges between or among two or more functions of a product, with the appropriate sign factor according to the parity of the permutation.

Following the same elementary decomposition rules, we also find

$$\chi_n^{(123)}(a_1a_2a_3p_4\cdots p_n \mid h_1\cdots h_n)=\langle\phi \mid \psi_{h_1}^\dagger\cdots\psi_{h_n}^\dagger\psi_{p_n}\cdots\psi_{p_4}e^{-S}\psi_{a_3}\psi_{a_2}\psi_{a_1} \mid \Psi\rangle$$
$$=\delta_{n,3}\mathcal{A}(a \mid h)[\delta(a_1-h_1)\delta(a_2-h_2)\delta(a_3-h_3)]$$
$$+\mathcal{A}(a \mid h)[\delta(a_1-h_1)\delta(a_2-h_2)S_{n-2}(a_3p_4\cdots p_n \mid h_3\cdots h_n)]$$
$$+\mathcal{A}(a \mid h)[\delta(a_1-h_1)F_{n-1}^{(12)}(a_2a_3p_4\cdots p_n \mid h_2\cdots h_n)]$$
$$+F_n^{(123)}(a_1a_2a_3p_4\cdots p_n \mid h_1\cdots h_n)\ , \tag{A5}$$

where

$$F_n^{(123)}(a_1a_2a_3p_4\cdots p_n \mid h_1\cdots h_n)=\langle\phi \mid \psi_{h_1}^\dagger\cdots\psi_{h_n}^\dagger\psi_{p_n}\cdots\psi_{p_4}\{[\psi_{a_3},[\psi_{a_2},[\psi_{a_1},S]]]+[\psi_{a_3},S][\psi_{a_2},[\psi_{a_1},S]]$$
$$+[\psi_{a_3},[\psi_{a_2}S]][\psi_{a_1},S]+[\psi_{a_2},S][\psi_{a_3},[\psi_{a_1},S]]$$
$$+[\psi_{a_3},S][\psi_{a_2},S][\psi_{a_1},S]\} \mid \phi\rangle$$
$$=\mathcal{A}(p \mid h)\{S_n(a_1a_2a_3p_4\cdots p_n \mid h_1\cdots h_n)$$
$$+\sum_{n_1}[S_{n_1}(a_1a_2p_4\cdots p_{n_1+1} \mid h_1\cdots h_{n_1})S_{n-n_1}$$
$$\times(a_3p_{n_1+2}\cdots p_n \mid h_{n_1+1}\cdots h_n)$$
$$+(a_2\leftrightarrow a_3)+(a_3\leftrightarrow a_1,a_1\leftrightarrow a_2,a_2\leftrightarrow a_3)]$$
$$+\sum_{n_1n_2}S_{n_1}(a_1p_4\cdots p_{n_1+2} \mid h_1\cdots h_{n_1})S_{n_2}$$
$$\times(a_2p_{n_1+2}\cdots p_{n_1+n_2+4} \mid h_{n_1+1}\cdots h_{n_1+n_2})$$
$$\times S_{n-n_1-n_2}(a_3p_{n_1+n_2+5}\cdots p_n \mid h_{n_1+n_2+1}\cdots h_n)\}\ . \tag{A6}$$

Various special cases of these formulas are applied in Sec. IV.

APPENDIX B: STATE INDEPENDENCE OF THE EFFECTIVE INTERACTIONS

The immediate aim of this appendix is to show that in Eq. (3.12) of the text,

$$\langle A \mid \psi_a^\dagger\psi_b^\dagger\psi_d\psi_c \mid G\rangle=\langle G \mid \psi_a^\dagger\psi_b^\dagger Q_A\psi_d\psi_c \mid G\rangle$$
$$+\langle G \mid [Q_A,\psi_a^\dagger\psi_g^\dagger]\psi_d\psi_c \mid G\rangle\ , \tag{B1}$$

the second term is $O(N^{-1})$ compared to the first. Here Q_A is defined by the equation

$$\mid A\rangle=Q_A^\dagger \mid G\rangle\ . \tag{B2}$$

We shall carry out the demonstration in a form which is strictly valid in the presence of a hard core and for a more general class of matrix elements than the left-hand side of (B1).

Reverting to a coordinate space representation (and

neglecting spin and charge), we require for any two eigenstates $|A\rangle$, $|B\rangle$ and for any operator O which is a finite polynomial in the ψ and $\psi^\dagger$ that

$$\langle A | \psi^\dagger_{x_1}\psi^\dagger_{x_2} O | B\rangle = 0 \quad \text{if } |\mathbf{x}_1-\mathbf{x}_2| < r_c \ , \tag{B3}$$

because this quantity is a building block for observables. Now, as in (B1), we write for $|B\rangle = |G\rangle$

$$\langle G | [Q_A, \psi^\dagger_{x_1}\psi^\dagger_{x_2}] O | G\rangle = \langle A | \psi^\dagger_{x_1}\psi^\dagger_{x_2} O | G\rangle - \langle G | \psi^\dagger_{x_1}\psi^\dagger_{x_2} Q_A O | G\rangle \ . \tag{B4}$$

Since both terms on the right-hand side of (B4) are finite and of the form (B3), it follows that the left-hand side is finite and vanishes for $|\mathbf{x}_1-\mathbf{x}_2| < r_c$. This requirement puts definite restrictions on the form of the operator Q_A. Its general form is

$$Q_A = \int dx\, \psi^\dagger_x \psi_x q^*_{A1}(x\,|\,x) + \int dx\, dx'\, \psi^\dagger_x \psi^\dagger_{x'} \psi_{x'} \psi_x q^*_{A2}(xx'\,|\,xx') + \cdots \ , \tag{B5}$$

i.e., it is a functional only of the local density, $\psi^\dagger_x \psi_x$. One verifies on the one hand that this form leads to the commutator

$$\langle G | [Q_A, \psi^\dagger_{x_1}\psi^\dagger_{x_2}] O | G\rangle = \langle G | \psi^\dagger_{x_1}\psi^\dagger_{x_2} [q^*_{A1}(x_1\,|\,x_1) + q^*_{A1}(x_2\,|\,x_2)] O | G\rangle + \cdots \ , \tag{B6}$$

where each term of the sum conforms to the structure (B3). On the other hand, any effort to introduce a nonlocal density dependence will violate this same property.

This point may be made obvious by the following remarks: Let $\phi_i(x_1 \cdots x_N)$, $i=1,2$ be two completely antisymmetric N-body wave functions with the hard-core property $\phi_i = 0$ for $|\mathbf{x}_i - \mathbf{x}_j| < r_c$. Then the two wave functions can obviously be related by the equation

$$\phi_2(x_1 \cdots x_N) = q_{21}(x_1 \cdots x_N)\phi_1(x_1 \cdots x_N) \ , \tag{B7}$$

where q_{21} is a finite symmetric function of its arguments. Equations (B5) and (B7) are equivalent statements, if for 1 one reads G and for 2 one reads A.

To complete our discussion, we first remark that every term on the right-hand side of (B6) is of the same order in N. It suffices then to compare $\langle G | \psi^\dagger_{x_1}\psi^\dagger_{x_2} Q_A O | G\rangle$ with

$$\langle G | \psi^\dagger_{x_1}\psi^\dagger_{x_2} [q^*_{A1}(x_1\,|\,x_1) + q^*_{A1}(x_2\,|\,x_2)] O | G\rangle \ .$$

Note that Q_A is an operator of order unity since it carries a normalized ket into another normalized ket. From (B5) it follows that $q_{A1}(x\,|\,x)$ is $O(N^{-1})$. Thus the second term of (B1) is $O(N^{-1})$ compared to the first one, and this result is not confined to this special choice $O = \psi_d \psi_c$. Our conclusion is that for a large system, the effective interaction is state independent. For finite nuclei there may be non-negligible corrections, but this is as far as we wish to carry the current investigation.

We must also consider the derivation of Eq. (3.13). We have

$$\langle G | \psi^\dagger_a \psi^\dagger_b Q_A \psi_d \psi_c | G\rangle = \langle G | \psi^\dagger_a \psi^\dagger_b e^{-S^\dagger} I_{N-2} e^{S^\dagger} Q_A \psi_d \psi_c | G\rangle \ . \tag{B8}$$

Introducing I_{N-2} from Eq. (2.6) and also noting that we can write Q_A in particle-hole or shell-model form, namely as a polynomial in the operators $\psi^\dagger_h \psi_p$, it follows that

$$[Q_A, \psi_p] = [Q_A, \psi^\dagger_h] = 0 \ , \tag{B9}$$

so that we can shift $e^{S^\dagger}$ and Q_A together to act to the left on $\langle \phi |$ and turn it into $\langle A |$. At this point the derivation of (3.13) shadows that of (3.8).

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