Unification of Brueckner Theory and HFB Theory

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A cluster expansion for the expectation value of operators with correlated wave functions is presented. A variational approach to the Brueckner theory with occupation probabilities is generalized and HFB theory incorporated.

1. Introduction

The usual approach to the Brueckner theory is to derive the expression for the ground-state energy of a many-particle system from perturbation theory. By a partial summation of Goldstone diagrams, the Bethe-Goldstone equation defining the Brueckner two-body G-matrix is obtained. A refined version of the Brueckner theory [1] uses true occupation probabilities for single particle levels.

Da Providencia and Shakin employed a variational approach to the Brueckner theory [2], using a correlated wave function of the following form:

$$\psi = e^S \Phi; \quad \Phi = \prod_{i=1}^{N} a_i^+ \,|\,0\,\rangle;$$
$$S = \tfrac{1}{2} \sum_{\substack{mn > N \\ ij \leq N}} C_{mn,ij}\, a_m^+ a_n^+ a_j a_i. \tag{1}$$

With the help of a partially summed cluster expansion for the expectation value $\langle \psi \,|\, H \,|\, \psi \rangle / \langle \psi \,|\, \psi \rangle$ of the Hamiltonian H of the N-particle system and a variation of the C-coefficients they arrived at a system of equations, which in the case of infinitely extended matter reduces to the Brueckner approximation of Brandow's theory [1, 3]. (The full formulation of this theory involves n-body operators in the definition of S.)

Wave functions of the form (1) including n-body operators in S have been investigated for the first time by Coester and later on by Kümmel and Lührmann [4—9]. (See also Ref. [10] for the case that S is a general two-body operator.)

In this paper a cluster expansion is presented dealing with general quasi-particle creation operators α^+ (fermion operators) in the correlated wave function instead of single particle operators a^+, a,

including the wave function (1) as a special case. Our cluster expansion proceeds in terms of the C-coefficients rather than in terms of cluster integrals [11—14], which themselves are polynomials of the C-coefficients. The cluster integrals of higher than second order, being complicated functions of the C-coefficients, are neglected in [2]. In the case of an infinite system, third order cluster integrals along with a 3-body operator part in S are considered in [15], where the 3-body Bethe-Faddeev equation is obtained after an appropriate approximation. Within our approach a wider class of diagrams contributing to the expectation value of H is summed up within the Brueckner-scheme, especially nonvanishing occupation probabilities for particle states above the Fermi sea are introduced. This generalization of the standard cluster expansion, which treats unoccupied and occupied single particle states "democratically" arises naturally in our quasi-particle formulation and is a necessary first step for incorporating the HFB theory into a Brueckner-scheme.

Minimizing the partial sum of diagrams with respect to the C-coefficients, we obtain a system of equations which can be recognized as generalized Brueckner theory, if we define the quasi-particle operators α, α^+ by means of a Hartree-Fock-Bogoljubov (HFB) transformation

$$a_p = \sum_q (A_{pq}\,\alpha_q + \overset{*}{B}_{pq}\,\alpha_q^+);$$
$$\alpha_p^+ = \sum_q (A_{qp}\,a_q^+ + B_{qp}\,a_q). \tag{2}$$

In addition, we obtain a generalized equation for the A, B-matrices which includes the minimum condition of HFB theory [16] in the special case $C = 0$.

The need for such a unification of the HFB theory and the Brueckner theory is motivated from the fact that one should have a microscopic theory

(starting with realistic N-N forces) for nuclei, where pairing effects are known to be important (e.g. Ca-Isotopes). Such a theory has been formulated up to now only for infinite systems using, however, the method of correlated-basis-functions [17].

2. The Cluster Expansion and Linked Cluster Theorem

For a given set of fermionoperators α_a, α_a^+ the quasi-particle vacuum Φ (with normalization $\langle \Phi | \Phi \rangle = 1$) is defined by

$$\alpha_a | \Phi \rangle = 0 \quad \text{for all } a.$$

The correlated wave function is written as:

$$\psi = e^S \Phi, \tag{3}$$

$$S = \frac{1}{2!} \sum_{a_1 a_2} C_{a_1 a_2} \alpha_{a_1}^+ \alpha_{a_2}^+ + \cdots$$

$$\cdots + \frac{1}{p!} \sum_{a_1 \ldots a_p} C_{a_1 \ldots a_p} \alpha_{a_1}^+ \cdots \alpha_{a_p}^+ + \cdots = \sum_{r=2}^{\infty} C^r,$$

where C^r denotes the operator part of S with r quasi-particle creation operators. Without loss of generality the C-coefficients can be antisymmetriz-ed with respect to the a-indices. The power series of e^S yields:

$$e^S = \sum_{i=0}^{\infty} F_i;$$

$$F_i = \sum_{p=1}^{\infty} \sum_{\substack{\mu_1 \leq \cdots \leq \mu_p \\ \mu_1 + \cdots + \mu_p = i}} \frac{1}{k_1! \ldots k_p!} C^{\mu_1} \ldots C^{\mu_p},$$

where $k_1, \ldots, k_p$ denotes the number of equal fig-ures in the p-tupel $(\mu_1, \ldots, \mu_p)$ respectively.

The unnormalized expectation value of a general operator Q, written with quasi-particle operators in normal order

$$Q = \sum_{m,n=0}^{\infty} \frac{1}{m!} \cdot \frac{1}{n!} \sum_{\substack{b_1 \ldots b_m \\ b_1' \ldots b_n'}}$$

$$\cdot q_{b_1 \ldots b_m, b_1' \ldots b_n'}^{m,n} \alpha_{b_1}^+ \cdots \alpha_{b_m}^+ \alpha_{b_n'} \cdots \alpha_{b_1'},$$

where the coefficients $q_{b,b'}^{m,n}$ are antisymmetrized in the b- and b'-indices, reads:

$$\tilde{Q} = \langle \Phi | e^{S^+} Q e^S | \Phi \rangle = \sum_{ij=0}^{\infty} \langle \Phi | F_i^+ Q F_j | \Phi \rangle. \tag{4}$$

Using the Wick-rule in the evaluation of each term in Eq. (4), it is now straightforward to construct diagrams D and diagram-rules such that $\tilde{Q}$ can be written as the sum of all contributions from all (topologically different) diagrams

$$\tilde{Q} = \sum_{D \in A} \tilde{Q}_D; \quad A := \text{set of all diagrams}.$$

The structure of these diagrams (examples are given in Fig. 1–6) and the explicit diagram-rules are presented in the appendix. The main advantage of this diagrammatic language is that a linked cluster theorem holds, saying that the division of Q through the norm cancels all unlinked diagrams, so that we have the linked expansion

$$\frac{\langle \psi | Q | \psi \rangle}{\langle \psi | \psi \rangle} = \sum_{D \in L} \tilde{Q}_D; \quad \begin{array}{l} L := \text{set of linked} \\ \text{diagrams}. \end{array}$$

(a)   (b)
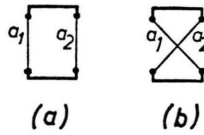
Fig. 1. Diagram (a) contributes to the norm $\langle \psi | \psi \rangle$ with

$$\langle \Phi | \frac{1}{2!} \overset{*}{C}_{a_1 a_2} \alpha_{a_2} \alpha_{a_1} \frac{1}{2!} C_{a_1 a_2} \alpha_{a_1}^+ \alpha_{a_2}^+ | \Phi \rangle$$

$$= \frac{1}{2!} \overset{*}{C}_{a_1 a_2} \cdot \frac{1}{2!} C_{a_1 a_2}.$$

The contribution of (b) is

$$\langle \Phi | \frac{1}{2!} \overset{*}{C}_{a_1 a_2} \alpha_{a_2} \alpha_{a_1} \frac{1}{2!} C_{a_2 a_1} \alpha_{a_2}^+ \alpha_{a_1}^+ | \Phi \rangle$$

$$= - \frac{1}{2!} \overset{*}{C}_{a_1 a_2} \cdot \frac{1}{2!} C_{a_2 a_1} = \frac{1}{2!} \overset{*}{C}_{a_1 a_2} \cdot \frac{1}{2!} C_{a_1 a_2}$$

and thus equal to that of (a).
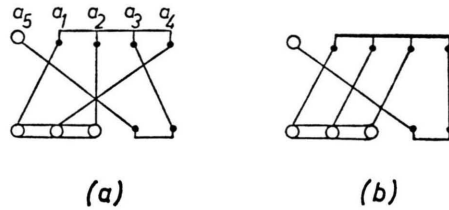

(a)   (b)

Fig. 2. Diagrams contributing to the unnormalized expecta-tion value of $q^{3,1}$.
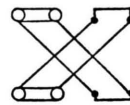

Fig. 3. A linked diagram, although topologically discon-nected.
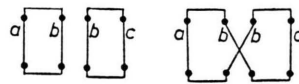

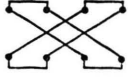Fig. 4. Two diagrams which violate the exclusion principle and yield opposite contributions.

Fig. 5 Diagram resulting from Fig. 4 (a) by permutation of upper or lower links.

Fig. 6. Diagram including the two diagrams of Figure 2.

3. Definition of the Generalized Brueckner Theory

We now specify the fermion operators α, α^+ as being defined by the HFB-transformation (2). The Hamiltonian H with two-body interaction v

$$H = T + V = \sum_{pq} t_{pq} a_p^+ a_q$$
$$+ \tfrac{1}{4} \sum_{pqrs} v_{pq,rs} a_p^+ a_q^+ a_s a_r,$$
$$v_{pq,rs} = \langle pq | V | rs \rangle, \quad t_{pq} = \langle p | T | q \rangle,$$
$$|ab\rangle = a_a^+ a_b^+ |0\rangle,$$

is expressed by normal ordered fermion operators

$$H = H^{0,0} + \sum_{a_1 a_2} \left(\frac{1}{2!} H^{0,2}_{a_1 a_2} \alpha_{a_2} \alpha_{a_1} + H^{1,1}_{a_1' a_2} \alpha_{a_1}^+ \alpha_{a_2} + \frac{1}{2!} H^{2,0}_{a_1 a_2} \alpha_{a_1}^+ \alpha_{a_2}^+ \right)$$
$$+ \sum_{a_1 a_2 a_3 a_4} \left(\frac{1}{4!} H^{0,4}_{a_1' a_2 a_3 a_4} \alpha_{a_4} \alpha_{a_3} \alpha_{a_2} \alpha_{a_1} + \frac{1}{3!} H^{1,3}_{a_1, a_2 a_3 a_4} \alpha_{a_1}^+ \alpha_{a_4} \alpha_{a_3} \alpha_{a_2} + \frac{1}{2!\,2!} H^{2,2}_{a_1 a_2, a_3 a_4} \alpha_{a_1}^+ \alpha_{a_2}^+ \alpha_{a_4} \alpha_{a_3} \right.$$
$$\left. + \frac{1}{3!} H^{3,1}_{a_1 a_2 a_3, a_4} \alpha_{a_1}^+ \alpha_{a_2}^+ \alpha_{a_3}^+ \alpha_{a_4} + \frac{1}{4!} H^{4,0}_{a_1 a_2 a_3 a_4} \alpha_{a_1}^+ \alpha_{a_2}^+ \alpha_{a_3}^+ \alpha_{a_4}^+ \right),$$

where the coefficients $H^{i,j}_{a_1 \ldots a_i, b_1 \ldots b_j}$ are antisymmetrized in the a- and b-indices, respectively, and by reason of $H^+ = H$ fulfill the relations:

$$H^{0,2}_{a_1 a_2} = \overset{*}{H}^{2,0}_{a_1 a_2}; \quad H^{1,1}_{a_1, a_2} = \overset{*}{H}^{1,1}_{a_2, a_1}; \quad H^{0,4}_{a_1 a_2 a_3 a_4} = \overset{*}{H}^{4,0}_{a_1 a_2 a_3 a_4}; \quad H^{1,3}_{a_1, a_2 a_3 a_4} = \overset{*}{H}^{3,1}_{a_2 a_3 a_4, a_1}; \quad H^{2,2}_{a_1 a_2, a_3 a_4} = \overset{*}{H}^{2,2}_{a_3 a_4, a_1 a_2}.$$

After introducing the density matrix [16]

$$\varrho_{ab} = \overset{*}{\varrho}_{ba} = \langle \Phi | a_b^+ a_a | \Phi \rangle = \sum_p \overset{*}{B}_{ap} B_{bp}$$

and the pair function

$$\varkappa_{ab} = -\varkappa_{ba} = \langle \Phi | a_a a_b | \Phi \rangle = \sum_p A_{ap} \overset{*}{B}_{bp}$$

the antisymmetrized $H_{i,j}$-coefficients can be written:

$$H^{0,0} = \sum_{ab} t_{ab} \varrho_{ba} + \tfrac{1}{2} \sum_{abcd} v_{ab,cd} \varrho_{ca} \varrho_{db} + \tfrac{1}{4} \sum_{abcd} v_{ab,cd} \overset{*}{\varkappa}_{ba} \varkappa_{dc},$$

$$H^{1,1} = \sum_{a_1 a_2} \left[\sum_{ab} t_{ab} (\overset{*}{A}_{aa_1} A_{ba_2} - B_{aa_2} \overset{*}{B}_{ba_1}) + \sum_{abcd} v_{ab,cd} \right.$$
$$\left. \cdot (\overset{*}{A}_{aa_1} A_{ca_2} \varrho_{db} - \overset{*}{B}_{ca_1} B_{aa_2} \varrho_{db} + \tfrac{1}{2} \overset{*}{A}_{aa_1} B_{ba_2} \varkappa_{dc} + \tfrac{1}{2} \overset{*}{B}_{da_1} A_{ca_2} \overset{*}{\varkappa}_{ba}) \right] \alpha_{a_1}^+ \alpha_{a_2},$$

$$H^{0,2}_{a_1 a_2} = \sum_{ab} t_{ab} (A_{ba_1} B_{aa_2} - A_{ba_2} B_{aa_1}) + \tfrac{1}{2} \sum_{abcd} v_{ab,cd}$$
$$\cdot (A_{da_2} A_{ca_1} \overset{*}{\varkappa}_{ba} + B_{aa_2} B_{ba_1} \varkappa_{dc} + 2(A_{ca_1} B_{aa_2} - A_{ca_2} B_{aa_1}) \varrho_{db}),$$

$$H^{3,1}_{b_1 b_2 b_3, a_1} = \sum_{abcd} v_{ab,cd} (\overset{*}{A}_{ab_1} \overset{*}{A}_{bb_2} \overset{*}{B}_{db_3} A_{ca_1} + \overset{*}{A}_{ab_2} \overset{*}{A}_{bb_3} \overset{*}{B}_{db_1} A_{ca_1} + \overset{*}{A}_{ab_3} \overset{*}{A}_{bb_1} \overset{*}{B}_{db_2} A_{ca_1}$$
$$+ \overset{*}{A}_{db_1} \overset{*}{B}_{db_2} \overset{*}{B}_{cb_3} B_{ba_1} + \overset{*}{A}_{ab_2} \overset{*}{B}_{db_3} \overset{*}{B}_{cb_1} B_{ba_1} + \overset{*}{A}_{ab_3} \overset{*}{B}_{db_1} \overset{*}{B}_{cb_2} B_{ba_1}),$$

$$H^{2,2}_{a_1 a_2, a_1' a_2'} = \sum_{abcd} v_{ab,cd} (\overset{*}{A}_{aa_1} \overset{*}{A}_{ba_2} A_{ca_1'} A_{da_2'} + \overset{*}{B}_{da_1} \overset{*}{B}_{ca_2} B_{ba_1'} B_{aa_2'} + \overset{*}{A}_{aa_1} \overset{*}{B}_{ca_2} A_{da_1'} B_{ba_2'}$$
$$- \overset{*}{A}_{aa_2} \overset{*}{B}_{ca_1} A_{da_1'} B_{ba_2'} - \overset{*}{A}_{aa_1} \overset{*}{B}_{ca_2} A_{da_2'} B_{ba_1'} + \overset{*}{A}_{aa_2} \overset{*}{B}_{ca_1} A_{da_2'} B_{ba_1'}),$$

$$H^{0,4}_{a_1 a_2 a_3 a_4} = \tilde{v}_{a_1 a_2, a_4 a_3} + \tilde{v}_{a_4 a_3, a_1 a_2} + \tilde{v}_{a_4 a_1, a_2 a_3} + \tilde{v}_{a_1 a_3, a_2 a_4} + \tilde{v}_{a_2 a_4, a_1 a_3} + \tilde{v}_{a_2 a_3, a_4 a_1};$$

$$\tilde{v}_{a_4 a_3, a_1 a_2} = \tfrac{1}{4} \sum_{abcd} v_{ab,cd} (B_{aa_4} B_{ba_3} A_{da_2} A_{ca_1}).$$

We first discuss the standard Brueckner case resulting from the ansatz (1) for the wave function which is in our language given by the special transformation

$$\alpha_p = u_p a_p^+ + v_p a_p; \quad \alpha_p^+ = u_p a_p + v_p a_p^+; \quad u_p = 1 \quad \text{for} \quad p \leq N,$$
$$u_p = 0 \quad \text{for} \quad p > N; \quad v_p = 1 - u_p \quad (N := \text{particle number}).$$

(5)

Diagram contributions to $\langle \psi | Q | \psi \rangle / \langle \psi | \psi \rangle$ can now be divided into terms, where the summation indices run only over values below the Fermi sea ($\leq N$) or above the Fermi sea ($> N$). Diagrammatically this is represented by a downgoing (hole line) or upgoing (particle line) line. For example, the diagram of Fig. 7(a) is then the sum of the three diagrams in Figures 7(b), (c), (d).
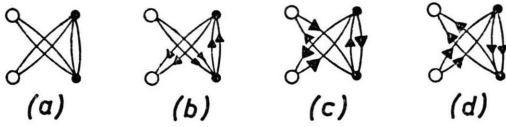

Fig. 7. Splitting of diagram (a) into diagrams with particle and hole lines.

(In our diagrammatic language the heavy dots in the upper sequence represent factors $\overset{*}{C}_{a_1' \dots a_\mu'}$ while the heavy dots in the lower sequence describe factors $C_{a_1 \dots a_\mu}$. Circles denote the matrix-elements $H^{i,j}_{a_1 \dots a_i, a_1' \dots a_j'}$; see appendix.)

The expression for the energy E of the system as evaluated in Ref. [2] expressed in our diagram language is given in Figure 8. The quadratic operator links indicate that only that part of $H^{1,1}$ containing the t-matrix elements is to be used. This is

due to the fact that there is no normal ordering procedure in the cluster expansion of [2]. There are two equivalent representations for E in Fig. 8, where $\gamma_{ij}' = \gamma_{ij} + \delta_{ij}$. Boxes with the γ symbols stand for an infinite partial sum of diagrams to be inserted there. γ is given by the diagrammatic equation of Figure 9. Algebraically Fig. 8 and Fig. 9 read, with
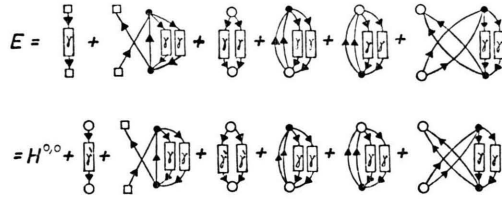
Fig. 8. Ground-state energy of Ref. [2] translated into our diagram language.
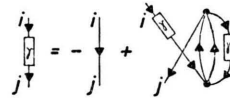
Fig. 9. Diagrammatic equation of Ref. [2] for γ_{ij} with reversed order of indices and opposite sign. The direct downgoing line represents $\delta_{ij} (i, j \leq N)$.

E denoting the approximated energy expectation value $\langle \psi | H | \psi \rangle / \langle \psi | \psi \rangle$:

$$
\begin{aligned}
E &= \sum_{ij \leq N} t_{ij} \gamma_{ij} + \tfrac{1}{2} \sum_{iji'j' \leq N} \langle i'j' | V + VS + S^+ V + S^+(T+V)S | ij \rangle \gamma_{i'i} \gamma_{j'j} \\
&= \sum_{ij \leq N} t_{ij} \gamma_{ij} + 2 \sum_{\substack{mn > N \\ iji'j' \leq N}} t_{mn} C_{nn', ij} \overset{*}{C}_{mn', ij} \gamma_{i'i} \gamma_{j'j} + \tfrac{1}{2} \sum_{\substack{ij \leq N \\ i'j' \leq N}} v_{i'j', ij} \gamma_{i'i} \gamma_{j'j} \\
&\quad + \tfrac{1}{2} \sum_{\substack{mn > N \\ iji'j' \leq N}} \overset{*}{C}_{mn, i'j'} v_{mn, ij} \gamma_{i'i} \gamma_{j'j} + \tfrac{1}{2} \sum_{\substack{iji'j' \leq N \\ mn > N}} v_{i'j', mn} C_{mn, ij} \gamma_{i'i} \gamma_{j'j} \\
&\quad + \tfrac{1}{2} \sum_{\substack{mnm'n' > N \\ ij \leq N}} v_{m'n', mn} \overset{*}{C}_{m'n', i'j'} C_{mn, ij} \gamma_{i'i} \gamma_{j'j},
\end{aligned}
$$

(6)

$$
\gamma_{ij} = \delta_{ij} - 2 \cdot \sum_{\substack{mn > N \\ kk'i' \leq N}} \gamma_{ii'} \overset{*}{C}_{mn, jk'} \gamma_{k'k} C_{mn, i'k}.
$$

(7)

The generalized Brueckner theory which we want to formulate within this paper is now given by the natural extension of the "standard" prescriptions expressed by Fig. 8, 9 to the case of general quasi-particles and is given diagrammatically by Fig. 10

Fig. 10. Extension of Fig. 8 to a sum of a wider class of diagrams.

and Figure 11. Since now particles and holes cannot be distinguished, we have to treat equivalent lines "democratically", i.e. we are necessarily lead to sum up the wider class of diagrams given by Figs. 10 and 11. This is the simplest possible generalization of the Brueckner scheme (Fig. 8, 9) to quasi-particles. Note that also the γ-matrix is now defined for all indices (below and above the Fermi sea) and that the first two diagrams of Fig. 8 are now incorporated in one diagram involving γ'. It can be

Fig. 11. Generalized diagrammatic equation for γ.

shown, that the solution of the equation for γ (Fig. 11), obtained by iterations with $\gamma = 0$ as a starting point, is a Hermitean matrix. The algebraic equation corresponding to Fig. 11 reads:

$$\gamma_{a,b} = -\delta_{ab} + \frac{1}{3!} \sum_{\substack{a_1 a_2 a_3 a_4 \\ a_2' a_3' a_4'}} \gamma_{aa_1} C_{a_1 a_2 a_3 a_4} \gamma_{a_2' a_2} \gamma_{a_3' a_3} \gamma_{a_4' a_4} \overset{*}{C}_{ba_2' a_3' a_4'} . \tag{8}$$
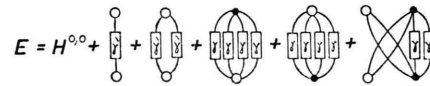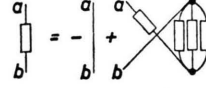
(The factor 1/3! is necessary to avoid overcounting of diagrams.) The algebraic expression for the energy (Fig. 10)

$$E = H^{0,0} + \sum_{a_1 a_2} H^{1,1}_{a_1, a_2} \gamma'_{a_2 a_1} + \frac{1}{2!} \sum_{abcd} H^{2,2}_{ab,cd} \gamma'_{ca} \gamma'_{db}$$

$$+ \frac{1}{4!} \sum_{\substack{a_1 a_2 a_3 a_4 \\ a_1' a_2' a_3' a_4'}} (H^{4,0}_{a_1 a_2 a_3 a_4} \overset{*}{C}_{a_1' a_2' a_3' a_4'} + H^{0,4}_{a_1' a_2' a_3' a_4'} C_{a_1 a_2 a_3 a_4}) \gamma_{a_1' a_1} \gamma_{a_2' a_2} \gamma_{a_3' a_3} \gamma_{a_4' a_4}$$

$$+ \frac{1}{8} \sum_{\substack{a_1 a_2 a_3 a_4 \\ a_1' a_2' a_3' a_4'}} H^{2,2}_{a_3' a_4', a_3 a_4} \overset{*}{C}_{a_1' a_2' a_3' a_4'} \gamma_{a_1' a_1} \gamma_{a_2' a_2} C_{a_1 a_2 a_3 a_4}$$

is a real quantity, if γ is Hermitean. To minimize E with respect to variations of C and $\overset{*}{C}$ the subsidiary condition (8) on C, $\overset{*}{C}$ is taken into account by Lagrange multipliers ε_{ab}:

$$F = E + \sum_{ab} \varepsilon_{ba}$$

$$\cdot \left(\gamma_{ab} + \delta_{ab} - \frac{1}{3!} \sum_{\substack{a_1 \ldots a_4 \\ a_2' \ldots a_4'}} \gamma_{aa_1} C \gamma \gamma \gamma C^* \right).$$

We have to express F as a function of $C_{a_1 a_2 a_3 a_4}$ with $a_1 < a_2 < a_3 < a_4$ with the help of a sum over permutations $\pi \in S_4$, in order to take into account the dependence of the C-coefficients due to antisymmetry. Since the wave function (3) is generally no eigenstate of the particle number operator

$$N_{op} = \sum_a a_a^+ a_a = N^{0,0} + \frac{1}{2} \sum_{pq} N^{0,2}_{qp} \alpha_p \alpha_q$$

$$+ \sum_{pq} N^{1,1}_{p,q} \alpha_p^+ \alpha_q + \frac{1}{2} \sum_{pq} N^{2,0}_{pq} \alpha_p^+ \alpha_q^+ ,$$

$$N^{0,0} = \sum_{ap} \overset{*}{B}_{ap} B_{ap},$$

$$N^{1,1}_{p,q} = \sum_a (\overset{*}{A}_{ap} A_{aq} - \overset{*}{B}_{ap} B_{aq}),$$

$$N^{0,2}_{qp} = 2 \sum_a A_{aq} B_{ap}, \quad N^{2,0}_{pq} = 2 \sum_a \overset{*}{A}_{ap} \overset{*}{B}_{aq},$$

we demand the expectation value

$$\langle \psi | N_{op} | \psi \rangle / \langle \psi | \psi \rangle$$

to be equal to N. This gives rise to the additional subsidiary condition

$$N^{0,0} + \sum_{\mu\nu} N^{1,1}_{\nu, \mu} \gamma'_{\mu\nu} - N = 0, \tag{9}$$

which is taken into account with the help of the Lagrange parameter ξ. By differentiation of

$$F + \xi (N^{0,0} + \sum_{pq} N^{1,1}_{p,q} \gamma'_{qp} - N)$$

with respect to γ, we obtain:

$$\varepsilon_{\nu\mu} = -H^{1,1}_{\nu, \mu} - \xi N^{1,1}_{\nu, \mu} - \sum_{ac} H^{2,2}_{\nu a, \mu c} \gamma'_{ca} - \sum_{\substack{a_1 a_2 a_3 \\ a_1' a_2' a_3'}} \left(\frac{1}{4} H^{2,2}_{a_2' a_3', a_2 a_3} \overset{*}{C}_{\mu a_1' a_2' a_3'} C_{\nu a_1 a_2 a_3} \gamma_{a_1' a_1} \right. \tag{10}$$

$$+ \left[-\frac{1}{3!} (H^{4,0}_{\nu a_1 a_2 a_3} \overset{*}{C}_{\mu a_1' a_2' a_3'} + H^{0,4}_{\mu a_1' a_2' a_3'} C_{\nu a_1 a_2 a_3}) + \frac{1}{(3!)^2} A \left(\sum_b \varepsilon_{b\mu} C^*_{ba_1' a_2' a_3'} \right) C_{\nu a_1 a_2 a_3} \right] \gamma_{a_1' a_1} \gamma_{a_2' a_2} \gamma_{a_3' a_3} \right)$$

(A denotes the antisymmetrizing operator $\sum_{\pi \in S_4}(-1)^\pi \pi$ for the indices μ, a_1', a_2', a_3') and differentiation with respect to C leads to:

$$H^{0,4}_{a_1 a_2 a_3 a_4} = \frac{1}{6}\sum_{\pi \in S_4}(-1)^\pi \sum_b \varepsilon_{b a_{\pi(1)}} \overset{*}{C}_{b a_{\pi(2)} a_{\pi(3)} a_{\pi(4)}}$$
$$- \frac{1}{8}\sum_{\pi \in S_4}(-1)^\pi \sum_{\substack{a_3' a_4' \\ a_3'' a_4''}} H^{2,2}_{a_3' a_4', a_3'' a_4''} \overset{*}{C}_{a_{\pi(1)} a_{\pi(2)} a_3' a_4'} \gamma^{-1}_{a_3'' a_{\pi(3)}} \gamma^{-1}_{a_4'' a_{\pi(4)}}. \tag{11}$$

Inserting $H^{0,4}$ from (11) in (10) we obtain:

$$\varepsilon_{\nu\mu} = - H^{1,1}_{\nu,\mu} - \xi N^{1,1}_{\nu,\mu} - \sum_{ac} H^{2,2}_{\nu a, \mu c}\gamma'_{ca} + \frac{1}{4}\sum_{\substack{a_1 \ldots a_4 \\ a_1' \ldots a_4'}} H^{2,2}_{a_3' a_4', a_3 a_4}\overset{*}{C}_{a_1' a_2' a_3' a_4'}\gamma_{a_1' a_1}\gamma_{a_2' a_2}C_{a_1 a_2 \nu a_4}\gamma^{-1}_{a_3' \mu}$$
$$- \frac{1}{3!}\sum_{\substack{a_1 a_2 a_3 \\ a_1' a_2' a_3'}} H^{4,0}_{\nu a_1 a_2 a_3}\overset{*}{C}_{\mu a_1' a_2' a_3'}\gamma_{a_1' a_1}\gamma_{a_2' a_2}\gamma_{a_3' a_3}. \tag{12}$$

A Hermitean adjoint equation is obtained by differentiation with respect to $\overset{*}{C}$. $\varepsilon_{\nu\mu}$ is not Hermitean, whereas $\varepsilon\gamma$ is Hermitean and the relation $\varepsilon\gamma = \gamma\varepsilon^+$ applies similar to [2]. If the Eqs. (8), (11) and (12) are fulfilled by the C- and γ-coefficients, F becomes the minimum value of the energy E:

$$E_{\min} = H^{0,0} + \sum_{a_1 a_2} H^{1,1}_{a_1' a_2}\gamma'_{a_2 a_1} + \frac{1}{2}\sum_{\substack{a_1 a_2 \\ a_1' a_2'}} H^{2,2}_{a_1 a_2, a_1' a_2'}\gamma'_{a_1' a_1}\gamma'_{a_2' a_2} + \sum_a \varepsilon_{aa} + \sum_{a_1 a_2}\varepsilon_{a_1 a_2}\gamma_{a_2 a_1}$$
$$+ \frac{1}{4!}\sum_{\substack{a_1 a_2 a_3 a_4 \\ a_1' a_2' a_3' a_4'}} H^{4,0}_{a_1 a_2 a_3 a_4}\overset{*}{C}_{a_1' a_2' a_3' a_4'}\gamma_{a_1' a_1}\gamma_{a_2' a_2}\gamma_{a_3' a_3}\gamma_{a_4' a_4}. \tag{13}$$

Equations (8), (9), (11), (12) and (13) constitute our HFB-generalization of the Brueckner theory.

4. Structure of the Generalized Brueckner Equations

For the sake of comparison, we first reveal the structure of the standard Brueckner-scheme. Varying Eq. (6) with respect to the $C, \overset{*}{C}$-coefficients under inclusion of the subsidiary condition (7) through Lagrange multipliers ε_{ij} ($i, j \le N$), we obtain [2]:

$$E = \sum_{i \le N}\varepsilon_{ii} + \sum_{ij \le N} U_{ij}\gamma_{ij} + \frac{1}{2}\sum_{iji'j' \le N} v_{i'j', ij}\gamma_{i'i}\gamma_{j'j} + \frac{1}{2}\sum_{\substack{iji'j' \le N \\ mn > N}} v_{i'j', mn}C_{mn, ij}\gamma_{i'i}\gamma_{j'j}, \tag{14}$$

$$\varepsilon_{ij} = t_{ij} - \left(\sum_{\substack{i'j' \le N \\ mn > N}} \overset{*}{C}_{mn, ii'} v_{mn, jj'}\gamma_{i'j'} + \sum_{i'j' \le N} v_{ii', jj'}\gamma_{i'j'}\right) = t_{ij} + U_{ij},$$

$$\sum_{i'j' \le N}\langle mn | T + V | i'j'\rangle \gamma_{ii'}\gamma_{jj'} + \sum_{\substack{i'j' \le N \\ mn > N}}\langle mn | T + V | m'n'\rangle C_{m'n', i'j'}\gamma_{ii'}\gamma_{jj'}$$
$$- 2\sum_{ghkl \le N} C_{mn, gh}(\varepsilon_{ki}\delta_{lj} + \varepsilon_{lj}\delta_{ki})\gamma_{kg}\gamma_{lh} = 0 \quad (m, n > N).$$

For infinite systems the matrices γ_{ij} and ε_{ij} are diagonal because of momentum conservation and we obtain the standard Brueckner scheme involving Brueckner's G-matrix:

$$E = \sum_{i \le N} t_{ii} + \frac{1}{2}\sum_{ij \le N}\langle ij | G | ij\rangle(1 - \sum_{i'j' \le N}\varkappa_{ii'}\varkappa_{jj'}),$$

$$G = V + V(Q/e)G; \quad e = T + U - QTQ,$$
$$\varepsilon_i = t_i + U_i$$
$$= t_i + \sum_{j \le N}\langle ij | G | ij\rangle(1 - \sum_{j < N}\varkappa_{ij})$$

where $\varkappa_{ij} = \langle ij | S^+ S | ij\rangle$ are the wound integrals and the relation between G and S is given by

$$\langle ij | G(\varepsilon_i + \varepsilon_j) | ij\rangle = \langle ij | V + VS | ij\rangle.$$

In our case it is necessary to compare the system of Eqs. (8), (11), (12), (13) to the Eqs. (14) for finite number of particles; especially here our HFB-generalization is expected to be essential, when nuclear systems are treated (see however Ref. [17]). In the energy expression of Eq. (14) appears a $H^{2,2}$ term (the third one) and a $H^{4,0}$ term (the last one), which

compensate each other to a large extend for the case of potentials inducing short range correlations. In order to cast (13) into a similar form, we split the operators $H^{1,1}$ and $H^{2,2}$ into different parts, which in the case of (2) being a HF-transformation (well-defined value of N) can be written:

$$H^{1,1} = PH^{1,1}P + QH^{1,1}Q + QH^{1,1}P \\ + PH^{1,1}Q$$

in the single-quasi-particle space, where

$$P = \sum_{a \leq N} \alpha_a^+ |\Phi\rangle\langle\Phi| \alpha_a;$$
$$Q = \sum_{a > N} \alpha_a^+ |\Phi\rangle\langle\Phi| \alpha_a,$$

and

$$H^{2,2} = PH^{2,2}P + (1-P)H^{2,2}(1-P);$$
$$P = \frac{1}{2} \sum_{a,b \leq N} \alpha_a^+ \alpha_b^+ |\Phi\rangle\langle\Phi| \alpha_b \alpha_a$$

in the two-quasi-particle space. Thus the operators can be written:

$$PH^{1,1}P = \sum_{a_1 a_2} \left[-\sum_{ab} t_{ab} B_{aa_2} \overset{*}{B}_{ba_1} - \sum_{abcd} v_{ab,cd} \overset{*}{B}_{ca_1} B_{aa_2} \varrho_{db} \right] \alpha_{a_1}^+ \alpha_{a_2},$$

$$PH^{1,1}Q = \sum_{a_1 a_2} \left[\sum_{abcd} \tfrac{1}{2} v_{ab,cd} \overset{*}{B}_{da_1} A_{ca_2} \overset{*}{\varkappa}_{ba} \right] \alpha_{a_1}^+ \alpha_{a_2},$$

$$QH^{1,1}P = \sum_{a_1 a_2} \left[\sum_{abcd} \tfrac{1}{2} v_{ab,cd} \overset{*}{A}_{aa_1} B_{ba_2} \varkappa_{dc} \right] \alpha_{a_1}^+ \alpha_{a_2},$$

$$QH^{1,1}Q = \sum_{a_1 a_2} \left[\sum_{abcd} v_{ab,cd} \overset{*}{A}_{aa_1} A_{ca_2} \varrho_{db} + \sum_{ab} t_{ab} \overset{*}{A}_{aa_1} A_{ba_2} \right] \alpha_{a_1}^+ \alpha_{a_2}^+,$$

$$PH^{2,2}P = \frac{1}{2!\,2!} \sum_{\substack{a_1 a_2 \\ a_1' a_2'}} \left[\sum_{abcd} v_{ab,cd} (\overset{*}{B}_{da_1} \overset{*}{B}_{ca_2} B_{ba_1'} B_{aa_2'}) \right] \alpha_{a_1}^+ \alpha_{a_2}^+ \alpha_{a_2'} \alpha_{a_1'},$$

$$(1-P)H^{2,2}(1-P) = \frac{1}{2!\,2!} \sum_{\substack{a_1 a_2 \\ a_1' a_2'}} \left[\sum_{abcd} v_{ab,cd} (\overset{*}{A}_{aa_1} \overset{*}{A}_{ba_2} A_{ca_1'} A_{da_2'} + \overset{*}{A}_{aa_1} \overset{*}{B}_{ca_2} A_{da_1'} B_{ba_2'} \right.$$
$$\left. - \overset{*}{A}_{aa_2} \overset{*}{B}_{ca_1} A_{da_1'} B_{ba_2'} - \overset{*}{A}_{aa_1} \overset{*}{B}_{ca_2} A_{da_2'} B_{ba_1'} + \overset{*}{A}_{aa_2} \overset{*}{B}_{ca_1} A_{da_2'} B_{ba_1'} \right] \alpha_{a_1}^+ \alpha_{a_2}^+ \alpha_{a_2'} \alpha_{a_1'}.$$

These equations are maintained also in the case of a general HFB-transformation, although the P and Q operators are not defined in this case. The matrix elements of the operators are now specified with regard to a "smeared" Fermi surface. Writing $E_{\min}$ in the form: (indices omitted)

$$E_{\min} = (H^{0,0} + \sum PH^{1,1}P\delta + \tfrac{1}{2}\sum PH^{2,2}P\delta\delta) + \sum_a \varepsilon_{aa} + \sum (PH^{1,1}P + PH^{2,2}P\delta + \varepsilon)\gamma$$
$$+ \sum (QH^{1,1}Q + PH^{1,1}Q + QH^{1,1}P)\gamma' + \tfrac{1}{2}\sum PH^{2,2}P\gamma\gamma$$
$$+ \tfrac{1}{2}\sum (1-P)H^{2,2}(1-P)\gamma'\gamma' + \frac{1}{4!}\sum H^{4,0}C^+\gamma\gamma\gamma\gamma$$

all terms of the first bracket cancel each other, with the exception of the pair interaction contribution term $\tfrac{1}{4}\sum_{abcd} v_{ab,cd} \overset{*}{\varkappa}_{ba}\varkappa_{dc}$ of $H^{0,0}$. The second bracket reduces to

$$\sum_{a_1 a_2} \left[-\sum_{ab} (t_{ab} \overset{*}{B}_{ba_1} B_{aa_2}) + \varepsilon_{a_1 a_2} \right] \gamma_{a_2 a_1} = \sum_{a_1 a_2} [-T_{a_1 a_2} + \varepsilon_{a_1 a_2}] \gamma_{a_2 a_1}.$$

Defining

$$\tilde{\varepsilon}_{\nu\mu} = \varepsilon_{\nu\mu} + (QH^{1,1}Q + PH^{1,1}Q + QH^{1,1}P)_{\nu\mu} + \left(\sum (1-P)H^{2,2}(1-P)\gamma'\right)_{\nu\mu},$$

we obtain:

$$F = E_{\min} = \tfrac{1}{4}\sum v\overset{*}{\varkappa}\varkappa + \sum_a \tilde{\varepsilon}_{aa} + \sum (-T + \tilde{\varepsilon})\gamma + \tfrac{1}{2}\sum PH^{2,2}P\gamma\gamma$$
$$- \tfrac{1}{2}\sum (1-P)H^{2,2}(1-P)\gamma'\gamma' + \frac{1}{4!}\sum H^{4,0}C^+\gamma\gamma\gamma\gamma, \tag{15}$$

$$\tilde{\varepsilon} = T - \sum PH^{2,2}P\gamma + \tfrac{1}{4}\sum H^{2,2}\overset{*}{C}\alpha\alpha C\alpha^{-1} - \frac{1}{3!}\sum H^{4,0}\overset{*}{C}\alpha\alpha.$$

We recognize, that Eq. (15) has indeed a very similar structure compared to the standard theory, Eq. (14); there are single-particle terms involving U, respectively $\bar{\varepsilon} - T$, there are "hole-hole interaction" terms resulting from $v_{ij, i'j'}$, respectively $H^{2,2}$, and there are particle-hole terms ($v_{ij, mn}$, respectively $H^{4,0}$). Thus one may expect that in Eq. (15) a similar compensation takes place as in the standard case. A numerical investigation of this question should be of great interest.

In case that (2) is a HF-transformation with well-defined particle number N of Φ, the equations corresponding to Fig. 10, 11 result from the standard Brueckner scheme (Fig. 8, 9) by insertions of boxes with γ (or γ') symbols into some of the particle lines and adding diagrams of the type of the third and the last one of Fig. 8 with reversed direction of the lines joining the boxes. (Note that one has to redefine the $QH^{1,1}Q$-matrix elements as not to include the v-interaction part in order to account for the quadratic operator links in Figure 8). The corrections introduced by our extension are expected to be small, since the γ_{mi} with $m > N$, $i \leq N$ are zero and the γ_{mn} with $m, n > N$ are supposed to be near to δ_{mn}. An indication that this is the case is the reduced number of infinite summations in the definition of the γ_{mn} as compared to the definition of γ_{ij} with $i, j \leq N$. The definition of the γ_{mn} contains one more summation over hole states (indices below the Fermi sea) than the γ_{ij}. Therefore, comparing our linked cluster expansion with the Thouless expansion [18, 3], we recognize that γ_{mn} involves diagrams with one more hole line.

Also the other additional terms of Fig. 10 contain one or two more hole lines for the leading contributions (see Figures 7 b, c).

5. The generalized HFB-Equation

We now impose the expectation value

$$\tilde{H}' = \frac{\langle \Phi | e^{S^+}(H + \xi N_{op}) e^S | \Phi \rangle}{\langle \Phi | e^{S^+} e^S | \Phi \rangle}$$

to be stationary with respect to infinitesimal variations of Φ. The subsidiary condition is Equation (9). It can be shown by group-theoretical methods that any HFB-state Φ' may be represented as [19]

$$|\Phi'\rangle = e^{SB} | \Phi \rangle;$$
$$SB = C^{0,0} + \sum_{ab} C^{1,1}_{a,b} \alpha_a^+ \alpha_b + \tfrac{1}{2} \sum_{ab} C^{0,2}_{ab} \alpha_b \alpha_a$$
$$+ \tfrac{1}{2} \sum_{ab} C^{2,0}_{ab} \alpha_a^+ \alpha_b^+;$$
$$C^{0,0} = -\tfrac{1}{2} \sum_a u_{aa}; \quad C^{1,1}_{a,b} = u_{ab};$$
$$C^{0,2}_{ab} = v_{ba}; \quad C^{2,0}_{ab} = \tilde{v}_{ab},$$

where $u^+ = -u$ and $\tilde{v} = -v$ and u, v being independent, as is not the case for the A, B of Equation (2). The stationarity condition of $\tilde{H}'$ yields that the partial derivatives of the expression

$$E' = \frac{\langle \Phi | e^{SB^+} e^{S^+} H' e^S e^{SB} | \Phi \rangle}{\langle \Phi | e^{SB^+} e^{S^+} e^S e^{SB} | \Phi \rangle},$$
$$H' = H + \xi N_{op} \qquad (16)$$

with respect to SB, SB^+ vanish at $SB = SB^+ = 0$, i.e.: (Stationarity with respect to a variation of S is fulfilled, if Eqs. (8), (11) und (12) hold.)

$$\frac{\partial E'}{\partial SB^+}\bigg|_{\substack{SB=0 \\ SB^+=0}} = \frac{\partial E'}{\partial SB}\bigg|_{\substack{SB=0 \\ SB^+=0}} = 0 = \frac{\partial}{\partial SB} \frac{\langle \Phi | (1 + SB^+) e^{S^+} H' e^S (1 + SB) | \Phi \rangle}{\langle \Phi | (1 + SB^+) e^{S^+} e^S (1 + SB) | \Phi \rangle}\bigg|_{SB=SB^+=0}.$$

Since in this expression only the term $C^{2,0}$ of SB contributes, we arrive at

$$\frac{\partial}{\partial C^{2,0}_{\alpha_1 \alpha_2}} \langle \Phi | e^{S^+} H' e^S C^{2,0} | \Phi \rangle\bigg|_{C^{2,0}=0} = 0; \quad (a_1 < a_2),$$

which can also be obtained from (16) by replacing SB by $C^{2,0}$ and SB^+ by $(C^{2,0})^+ = -C^{0,2}$. This modified expectation value is a sum of linked diagram contributions. The partial derivatives of this sum with respect to $C^{2,0}$ at $C^{2,0} = C^{0,2} = 0$ must be zero. Only those diagrams with no $C^{0,2}$-link (no second order link in the upper sequence) and one $C^{2,0}$-link (one second order link in the lower sequence) need to be considered in the differentiation. An approximate expression for the sum of diagrams corresponding to our generalized Brueckner-approach and contributing to the differentiation is given by the diagrams of Fig. 12 with the algebraic expression:

Fig. 12. Approximate sum contributing to the differentiation of (16) with respect to $C^{2,0}$. ▶

$$\tilde{E} =$$
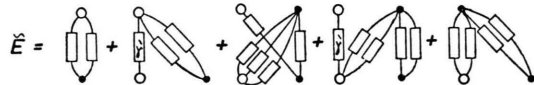
$$\tilde{E} = \sum_{\substack{a_1 a_2 \\ a_1' a_2'}} C_{a_1 a_2}\, \gamma_{a_1' a_1}\, \gamma_{a_2' a_2} \left\{ \frac{1}{2}\, H_{a_1' a_2'}'^{\,0,2} + \frac{1}{3!} \sum_{\substack{b_1 b_2 b_3 \\ b_1' b_2' b_3'}} H_{b_1 b_2 b_3,\, a_1'}^{3,1}\, \overset{*}{C}_{b_1' b_2' b_3' a_2'}\, \gamma_{b_1' b_1}\, \gamma_{b_2' b_2}\, \gamma_{b_3' b_3} \right.$$

$$\left. + \frac{1}{2} \sum_{b_1 b_1'} H_{b_1,\, b_1' a_1' a_2}^{1,3}\, \gamma_{b_1' b_1}' + \frac{1}{4} \sum_{\substack{a_3 a_4 \\ a_3' a_4'}} \overset{*}{C}_{a_3' a_4' a_1' a_2'}\, \gamma_{a_3' a_3}\, \gamma_{a_4' a_4} \left[H_{a_3 a_4}'^{\,2,0} + \sum_{b_1 b_1'} H_{b_1 a_3 a_4,\, b_1'}^{3,1}\, \gamma_{b_1' b_1}' \right] \right\}.$$

Minimizing $\tilde{E}$ with respect to independent $C_{a_1 a_2}$ and considering that $C_{a_1 a_2}$ is antisymmetric, we obtain:

$$H_{a_1 a_2}^{0,2} + \xi N_{a_1 a_2}^{0,2} + \sum_{b_1 b_1'} H_{b_1,\, b_1' a_1 a_2}^{1,3}\, \gamma_{b_1' b_1}'$$

$$+ \frac{1}{3!} \sum_{\substack{b_1 b_2 b_3 \\ b_1' b_2' b_3'}} (H_{b_1 b_2 b_3,\, a_1}^{3,1}\, \overset{*}{C}_{b_1' b_2' b_3' a_2} - H_{b_1 b_2 b_3,\, a_2}^{3,1}\, \overset{*}{C}_{b_1' b_2' b_3' a_1})\, \gamma_{b_1' b_1}\, \gamma_{b_2' b_2}\, \gamma_{b_3' b_3} \qquad (17)$$

$$+ \frac{1}{2} \sum_{\substack{a_3 a_4 \\ a_3' a_4'}} \overset{*}{C}_{a_3' a_4' a_1 a_2}\, \gamma_{a_3' a_3}\, \gamma_{a_4' a_4} \left[H_{a_3 a_4}^{2,0} + \xi N_{a_3 a_4}^{2,0} + \sum_{b_1 b_1'} H_{b_1 a_3 a_4,\, b_1'}^{3,1}\, \gamma_{b_1' b_1}' \right] = 0$$

for all a_1, a_2.

A Hermitian adjoint equation results from

$$\frac{\partial E'}{\partial SB^+}\bigg|_{SB = SB^+ = 0} = 0.$$

In the case of $C_{a_1 \ldots a_4} = 0$ ($\gamma' = 0$), (17) reduces to $H^{0,2} + \xi N^{0,2} = 0$, the minimum condition of HFB-theory. As in the case of HFB-theory the HFB-transformation (2) is not completely determined by (17), since a unitary transformation of single-particle states, which do not alter Φ, remains undetermined. The complete system of equations determining the "short range" part S and the "long range" part SB of the correlations in the wave function is given by the Eqs. (8), (9), (11), (12) and (17). These equations should be adequate to give a description of, e.g. the ground state energies of Ca-Isotopes, when using the full Reid potential. Up to now such calculations have been done only with the simplifying assumption that the standard HFB equations are valid for an "effective potential" given by a suitable Brueckner G-matrix.

In fact, Eq. (17) has a structure which makes plausible such a procedure, however a more refined justification can only be found by a detailed numerical investigation, which remains to be done in the future.

Appendix

This appendix is devoted to the exposition of our diagram language and diagram rules. Our definition of diagrams is inspired by the graphs used by da Providencia and similarly Schäfer in defining cluster integrals [11, 13, 14]. However, whereas those graphs do not allow to establish a linked-cluster theorem for the normalized expectation value of an operator or for the norm of the wave function our diagrams do, because of treating the indices above and below the Fermi sea in the same way. A general proof is given in [20].

Inserting the expressions for F_i, F_j and Q in Eq. (4) and extracting the C- and Q-coefficients from the expectation value, we obtain a sum, whose terms are products of factors

$$\frac{1}{\mu'!}\, \overset{*}{C}_{a_{1'} \ldots a'_{\mu'}}, \qquad \frac{1}{\mu!}\, C_{a_1 \ldots a_\mu},$$

one factor $(1/m!\, n!)\, q_{b, b'}^{m, n}$ and the remaining expectation value of quasiparticle operators:

$$\langle \Phi |\, \alpha_{a'_{(\mu_{1'} + \cdots + \mu'_{p'})}} \cdots \alpha_{a_{1'}} (\alpha_{b_1}^+ \ldots \alpha_{b_m}^+ \alpha_{b_{n'}} \ldots \alpha_{b_{1'}})$$
$$\cdot \alpha_{a_1}^+ \ldots \alpha_{(\mu_1 + \cdots + \mu_p)}^+ |\, \Phi \rangle. \quad (18)$$

A necessary condition for (18) not to vanish, is the equality of indices with stroke

$$(b_1', \ldots, b_n', a_1', \ldots, a'_{\mu_{1'} + \cdots + \mu'_{p'}}),$$

to a permutation of indices without stroke

$$(b_1, \ldots, b_m, a_1, \ldots, a_{\mu_1 + \cdots + \mu_p}).$$

Therefore, we can sum over the permutations $\pi \in S_{m + \mu_1 + \cdots + \mu_p}$ of the indices without stroke, instead of summing over the indices with stroke. Having suitably renamed the indices, the expectation value (18) is equal to $(+1)$ for $\pi = \mathrm{id}$ (id: identity) and (18) may be replaced by $(-1)^\pi$, provided that the set of $(b_1', \ldots, b_n')$-indices, being all unequal to each other, is included in the $(a_1, \ldots, a_{\mu_1 + \cdots + \mu_p})$-indices, being also all unequal, and pro-

vided that the set of unequal $(b_1, \ldots, b_m)$ is included in the set of unequal $(a'_1, \ldots, a'_{\mu'_1 + \cdots + \mu'_{p'}})$. Otherwise (18) vanishes. Every term of the sum (4) characterised by fixed values of n, m, i, j, p, p', $\mu_1, \ldots, \mu_p$, $\mu'_1, \ldots, \mu'_{p'}$, $a_1, \ldots, a_{\mu_1 + \cdots + \mu_p}$ and π can be assigned a diagram representing the contribution of that term to the sum. A factor $\dfrac{1}{\mu!} \overset{*}{C}_{a_1 \ldots a_\mu}$ is represented by a "link" with μ joining pieces for quasi-particle lines $a_1 \ldots a_\mu$. In the same way a factor $\dfrac{1}{\mu!} \overset{*}{C}^*_{a_1 \ldots a_\mu}$ is represented. Links representing C-coefficients are drawn in a lower sequence side by side, arranged with respect to the number of joining pieces from the left to the right, the links for the $\overset{*}{C}$-coefficients being arranged in the same manner in an upper sequence. Joining pieces with the same index in the lower and upper sequence are connected by a quasi-particle line (q.-p. line). Every joining piece in the lower sequence must be connected to one in the upper sequence, in order that the diagram contributes to $\tilde{Q}$. The topological character of the arrangement of the q.-p. lines is determined by the permutation π of the a-indices. To each different π corresponds a diagram with

corresponding permutation of the q.-p. lines at the upper or lower link-joining pieces. Two diagrams that contribute to the norm $\langle \psi | \psi \rangle$ $(Q = 1)$ are shown in Figure 1. Diagrams contributing to an unnormalized operator expectation value $\tilde{Q}$, Q being of the form

$$\frac{1}{m! \, n!} \sum_{b,b'} q^{m,n}_{b,b'} \, \alpha^+_{b_1} \ldots \alpha^+_{b_m} \alpha_{b_{n'}} \ldots \alpha_{b_{1'}},$$

have a special Q-link on the left side of the lower sequence preceeding the C-links, with m joining pieces for q.-p. lines $b_1 \ldots b_m$, and another Q-link on the left side of the upper sequence with n joining pieces for q.-p. lines $b'_1 \ldots b'_n$. Both Q-links together represent the factor $(1/m! \, n!) q^{m,n}_{b,b'}$. By reason of the argument following (18) the q.-p. annihilation part of the Q-operator (b'-indices) in the upper sequence and the q.-p. creation part of Q (b-indices) are connected to C, $\overset{*}{C}$-links in the lower and upper sequence, respectively. No diagrams with direct q.-p. line connections between the Q-links in the lower and upper sequence are allowed. Figure 2(a) shows an example for a diagram contributing to $\tilde{Q}$, for Q being of the type $q^{3,1}$. This diagram has the value:

$$\langle \Phi | \frac{1}{4!} \overset{*}{C}_{a_1 a_2 a_3 a_4} \alpha_{a_4} \alpha_{a_3} \alpha_{a_2} \alpha_{a_1} \frac{1}{3!} q^{3,1}_{a_1 a_4 a_2, a_5} \alpha^+_{a_1} \alpha^+_{a_4} \alpha^+_{a_2} \alpha_{a_5} \frac{1}{2!} C_{a_5 a_3} \alpha^+_{a_5} \alpha^+_{a_3} | \Phi \rangle$$

$$= \frac{1}{4!} \overset{*}{C}_{a_1 a_2 a_3 a_4} \frac{1}{3!} q^{3,1}_{a_1 a_4 a_2, a_5} \frac{1}{2!} C_{a_5 a_3} = \frac{1}{4!} \overset{*}{C}_{a_1 a_2 a_3 a_4} \frac{1}{3!} q^{3,1}_{a_1 a_2 a_4, a_5} \frac{1}{2!} C_{a_3 a_5}.$$

A diagram without indices at the q.-p. lines, is defined to be the sum of all topological identical diagrams with indices. The rules for the evaluation of the corresponding algebraic expression of a given diagram without indices are summarized here:

1. Attribute to each q.-p. line a general index and provide thereby the factors

$$\frac{1}{\mu'!} \overset{*}{C}_{a_{1'} \ldots a_{\mu'}}, \quad \frac{1}{\mu!} C_{a_1 \ldots a_\mu}$$

for the $\overset{*}{C}$-, C-links with indices.

2. Multiply by a factor $1/(k_1! \ldots k_p!)$, if there are $k_1 \ldots k_p$ C-links of the same type respectively in the lower sequence, (i.e. they have the same number of joining pieces), and a factor $1/(k'_1! \ldots k'_p!)$ for the $\overset{*}{C}$-links being of equal type in the upper sequence.

3. Multiply by a factor $1/(m! \, n!) q^{m,n}_{b_1 \ldots b_m, \, b_n \ldots b'_1}$ for the Q-links, where $b'_1 \ldots b'_n$ denote the q.-p. lines joining the upper Q-link and $b_1 \ldots b_m$ denote the lines joining the lower Q-link.

4. Sum over all indices of the product.

5. Multiply the sum by a sign which is given by the number z of interchanges of q.-p. lines at the upper and lower links necessary to obtain a diagram, where the q.-p. lines are drawn parallely from the Q-links to the nearest C-, $\overset{*}{C}$-links and the remaining lines connecting C-, $\overset{*}{C}$-links are also parallel. The sign is then $(-1)^z$.

This sign rule can be gathered from expectation value (18). (From

$$(b'_1 \ldots b'_n) = (a_1 \ldots a_n); \quad (b_1 \ldots b_m) = (a'_1 \ldots a'_m);$$
$$(a_{n+1} \ldots a_{\mu_1} + \cdots + \mu_p) = (a'_{m+1} \ldots a'_{\mu'_1 + \cdots + \mu'_{p'}})$$

follows that expression (18) equals $+1$.) The first diagram of Fig. 2 for example is transformed after 2 interchanges of q.-p. lines into the second diagram. Therefore, (a) has sign $(-1)^2 = +1$ like (b).

We define a diagram to be unlinked, if it consists of at least two parts, which are not connected to each other by q.-p. lines. A topologically disconnected diagram such as that shown in Fig. 3, is considered to be linked, because the Q-links are thought to be connected to one Q-vertex. In order to write the contribution of an unlinked diagram as a product of factors corresponding to the amounts of the linked parts, we have to abandon the Pauli exclusion principle in the expectation value (18), i.e. its value is defined to be $(-1)^\pi$, even if the unequality conditions for the indices following (18) are not satisfied. The resulting error is cancelled in the sum of the diagrams, since for each diagram with two q.-p. lines, having the same index, there is another diagram with those q.-p. lines at the joining pieces in the upper or equivalently lower sequence being interchanged. The contribution of this diagram has a reversed sign by reason of the factor $(-1)^\pi$ and the same absolute value. An example is provided by Figure 4. The diagram of Fig. 4(a) has the value

$$\frac{1}{2!} \cdot \frac{1}{2!} \cdot \frac{1}{2!} \overset{*}{C}_{bc} \cdot \frac{1}{2!} \overset{*}{C}_{ab} \cdot \frac{1}{2!} C_{ac} \cdot \frac{1}{2!} C_{bc},$$

whereas the contribution of Fig. 4(b) has the opposite value. The contribution of the diagram in Fig. 4(a) with indices absent, can now be written as follows:

$$\frac{1}{4} \left(\sum_{a_1 a_2 = 1}^{\infty} \frac{1}{2!} \overset{*}{C}_{a_1 a_2} \frac{1}{2!} C_{a_1 a_2} \right)^2 .$$

The same contribution is produced by the diagram of Fig. 5, where the links in the upper or equivalently lower sequence are interchanged.

From Fig. 1 we recognize that a permutation of q.-p. lines at the same link leads to a diagram with equal contribution, because the change in the sign $(-1)^\pi$ is the same as the change of sign in the antisymmetric C-, $\overset{*}{C}$- or Q-coefficient due to the corresponding permutation of the a-indices there. The sum of all these diagrams can be comprised in one new diagram with points representing the C-, $\overset{*}{C}$-links and circles for the Q-links. The diagrams of Fig. 2 are thus absorbed in the diagram of Figure 6.

Each diagram of the new kind can be represented by a matrix $z(i, j)$; $i = 0, 1, \ldots, p$; $j = 0, 1, \ldots, p'$, where $z(i, j)$ is the number of q.-p. lines connecting the i-th link in the lower sequence with the j-th link in the upper sequence ($i, j = 0: Q$-links; $i, j = 1, \ldots, p\, p': C$-, $\overset{*}{C}$-links). μ_i, μ_i' being the number of q.-p. lines joining-pieces for the i-th lower or upper link, $z(i, j)$ obeys the relations:

$$\sum_{i=0}^{p} z(i, j) = \mu_j'; \quad \sum_{j=0}^{p'} z(i, j) = \mu_i.$$

It can be shown, that the number of different diagrams of the old kind comprehended within one diagram of the new kind is

$$f = \prod_{j=0}^{p'} \prod_{i=0}^{p} \frac{\mu_j'! \cdot \mu_i!}{z(i, j)!}$$

$$= \frac{\mu_0'! \cdot \ldots \cdot \mu_{p'}'! \cdot \mu_0! \cdot \ldots \cdot \mu_p!}{z(0,0)!\, z(0,1)! \cdot \ldots \cdot z(0,p')!\, z(1,0)! \cdot \ldots \cdot z(p,p')!},$$

where $z(0, 0) = 0$ ($0! = 1$). Multiplying a representative diagram contribution of the old kind by f the factors $1/\mu!$ and $1/(m! \cdot n!)$ appearing after the diagram rules are cancelled. Dropping these factors and replacing f by

$$f' = 1 \Big/ \left[\prod_{i=0}^{p} \prod_{j=0}^{p'} z(i, j)! \right], \tag{19}$$

(a factor $1/z!$ for each direct connection with z q.-p. lines between two links) we obtain now somewhat modified diagram rules.

A further summing up of diagrams can be done by permuting C-, $\overset{*}{C}$-links of the same type in the upper or lower sequence together with their q.-p. lines connections. The diagrams of Fig. 13 are generated in this way from the diagram of Figure 13(a). We define a diagram like that of Fig. 13(a) to have a symmetry factor 1, if all diagrams generated this
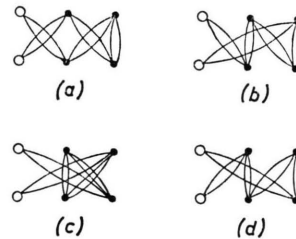

Fig. 13. Diagram (a) is defined to include all different diagrams created by link permutations, i.e. (a), (b), (c) and (d) shall represent the same diagram and are not considered to be different.

way are different. Their number is with inclusion of the original one $k_1! \cdot k_2! \cdot \ldots \cdot k_p! \cdot k_1'! \cdot \ldots \cdot k_p'!$ where the k's are those of the diagram rules. If n identical diagrams can be generated by different permutations in the lower and upper sequence, the symmetryfactor is defined as $1/n$ and is to be multiplied by the above number for determining the
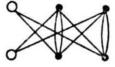

Fig. 14. Diagram with symmetry factor 1/2.

quantity of different diagrams. Therefore, the factor $1/(k_1! \ldots k_p! \cdot k_1' \ldots k_p'!)$ prescribed after the diagram rules can be omitted and be replaced by the symmetry factor $1/n$, thus including the sum of the contributions of all different diagrams, which are created by possible link permutations. In Fig. 14 a diagram is shown, which has symmetry

factor $1/2$, since interchanging of the first and third C- and $\overset{\bullet}{C}$-link leads to the same diagram.

For the special case, that the q.-p. operators are given by Eq. (5), the diagram of Fig. 7 (a) is separated into the diagrams of Fig. 7 (b), (c), (d). For these diagrams the factor (19) has to be replaced by

$$1 \Big/ \Big(\prod_{i,j=0} z_p(i,j)! \cdot \prod_{i,j=0} z_h(i,j)! \Big),$$

where $z_p(i, j)$ denotes the number of particle-lines and $z_h(i, j)$ of hole-lines connecting the i-th link in the lower sequence with the j-th link in the upper sequence. Similarly the factor $1/(m! \cdot n!)$ of the operator $q^{m,n}$ has to be replaced by

$$1/(m_p! \cdot m_h! \cdot n_p! \cdot n_h!),$$

where m_p, n_p is the number of indices in the lower and upper Q-link above the Fermi sea and m_h, n_h the number of indices below the Fermi sea

$$(m_p + m_h = m; \ n_p + n_h = n).$$

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