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Second-Quantization Formalism for Geminals

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A method of constructing second-quantization formalism on a set of orthonormal geminals (two-particle antisymmetric functions) is described. Instead of using an initial set of creation and annihilation operators with nontrivial commutation rules, the so-called ideal creation and annihilation operators, satisfying elementary Bose commutation rules, are used. The resulting Hamiltonian and an arbitrary observable can be uniquely expressed in terms of these ideal operators, playing now a rôle of dynamic variables. In order to simplify the evaluation of such ideal operators, a modified version of Feynman-Goldstone diagrammatic technique is used.

1. INTRODUCTION

One of the basic problems of up-to-date quantum chemical calculations of the electronic structure of atomic and/or molecular systems is the so-called correlation-energy problem. So far this problem has been usually solved within the framework of the independent-particle picture (restricted Hartree--Fock scheme, in most cases) plus some more or less efficient variational or perturbative techniques counting the correlation effects.[1,2] On the other hand, approaches have been developed and successfully applied which discard the independent-particle model from the outset, such as the geminal or more generally the group-function methods.[3–12] The main feature of these methods is that a trial wave function is expressed as the antisymmetrized product of two-particle antisymmetric functions — geminals; that is, the greatest part of the correlation effects is automatically included through this form of the trial wave function. Therefore, in order to obtain a unified first-principles theoretical treatment of the methods employing the geminals, we call attention to the second-quantization formalism, fully based on the fact that the geminals serve as a basis set for the construction of antisymmetric many-electron states spanning the Fock spaces. In this connection it is useful to recollect that in the framework of independent-particle schemes the second-quantization formalism offers a powerful machinery, which does not only facilitate their profound theoretical classification but also this formalism enables a »microscopic« formulation of many variational and perturbative techniques for correlation-energy calculations. A similar situation exists also for geminals, where the second-quantization formalism might be of value for further extension and generalization of methods based on the geminals. Especially

the many-body perturbation techniques are potentially applicable to highly precise correlation-energy calculations.

The purpose of this work is to develop a second-quantization formalism introduced onto an orthonormal set of geminals. In order to realize this program we used a method analogous to that developed by Dyson[13] for treating the problem of spin-wave interaction in ferromagnetism, and subsequently adapted by Girardeau[14] for the construction of second-quantization formalism for systems composed of composite particles. Dyson and Girardeau solved the problem of nontrivial commutation relations by introducing an ideal Fock space, in one-to-one correspondence with the physical Fock space spanned by all geminal-product states, in which the commutation relations were of elementary Bose form, and in which all calculations could be simply performed by transforming the Hamiltonian from the physical Fock space into an ideal Fock space. Recently, this approach has been successfully used by the author[15] for the construction of a second-quantization formalism on a set of nonorthogonal one-particle functions. To simplify and formalize our theoretical considerations leading to the construction of ideal operators, we use a modified version of Feynman-Goldstone diagrammatic technique[16]. It enables an advantageous classification of single terms contributing to the matrix elements from the ideal operators, and to formulate the so called »linked-cluster« theorems. From this standpoint, there are some common features between the present theory and the cluster-expansion method of Iwamoto and Yamada[17], widely used in microscopic theory of nuclear systems[18–21].

A diagrammatic method for the calculation of arbitrary matrix elements of an n-particle observable between the states represented by the antisymmetrized product of geminals of an arbitrary kind has been studied by Paldus *et al.*[22]. He started from the assumption that the geminals can be expanded in terms of an orthonormal set of one-particle functions and that the creation and annihilation operators are introduced onto this set of one-particle functions. The second-quantization formalism serves here only as a proper tool for the evaluation of matrix elements of an operator between two antisymmetrized products of geminals. Paldus did not try to construct the Hamiltonian in terms of the creation and annihilation operators defined on a set of geminals. In the present work the Feynman-Goldstone diagrammatic technique is employed as an auxiliary device to reach from the first principles the second-quantization formalism with respect to an orthonormal set of geminals.

2. BASIC THEORETICAL CONCEPTS

Considering a molecular system, its second-quantized Hamiltonian can be written in terms of electron-field creation and annihilation operators[23],

$$H = \int \mathrm{d}\, x\, \psi^{+}(x)\, h(x)\, \psi(x) + \frac{1}{2} \int \mathrm{d}\, x\, \mathrm{d}\, y\, \psi^{+}(x)\, \psi^{+}(y)\, g(x, y)\, \psi(y)\, \psi(x), \tag{1}$$

where $h(x)$ is the one-electron kinetic-energy operator plus electron-core attractive potentials, $g(x, y)$ is the two-electron interaction potential, and electron-field operators satisfy elementary Fermi anticommutation rules,

$$\begin{aligned} [\psi(x), \psi(y)]_{+} &= 0 = [\psi^{+}(x), \psi^{+}(y)]_{+}, \\ [\psi(x), \psi^{+}(y)]_{+} &= \delta(x - y). \end{aligned} \tag{2}$$

Let

$$\{\varphi_\alpha(x, y);\ \alpha = 1, 2, \ldots\} \tag{3}$$

be an orthonormal set of two-particle antisymmetric functions — geminals,

$$\int \mathrm{d}\, x\, \mathrm{d}\, y\, \varphi_\alpha^*(x, y)\, \varphi_\beta(x, y) = \delta_{\alpha\beta}, \tag{4a}$$

$$\varphi_\alpha(x, y) = -\varphi_\alpha(y, x). \tag{4b}$$

The corresponding creation and annihilation operators can be now defined as follows:

$$A_\alpha^+ = \frac{1}{\sqrt{2}} \int \mathrm{d}\, x\, \mathrm{d}\, y\, \varphi_\alpha(x, y)\, \psi^+(x)\, \psi^+(y), \tag{5a}$$

$$A_\alpha = \frac{1}{\sqrt{2}} \int \mathrm{d}\, x\, \mathrm{d}\, y\, \varphi_\alpha^*(x, y)\, \psi(y)\, \psi(x) = (A_\alpha^+)^+, \tag{5b}$$

where one can readily verify that these operators satisfy the following commutation relations

$$\begin{aligned} [A_\alpha, A_\beta]_- &= 0 = [A_\alpha^+, A_\beta^+]_-, \\ [A_\alpha, A_\beta^+]_- &= \delta_{\alpha\beta} + C_{\alpha\beta}. \end{aligned} \tag{6}$$

Here, the operator-valued quantity $C_{\alpha\beta}$ is determined by

$$C_{\alpha\beta} = 2 \int \mathrm{d}\, x\, \mathrm{d}\, y\, K_{\alpha\beta}(x, y)\, \psi^+(x)\, \psi(y), \tag{7a}$$

$$K_{\alpha\beta}(x, y) = \int \mathrm{d}\, t\, \varphi_\alpha^+(y, t)\, \varphi_\beta(t, x). \tag{7b}$$

Let $|\, 0\,\rangle$ be the normalized ($\langle\, 0 \,|\, 0\,\rangle = 1$) vacuum-state vector,

$$\psi(x)\, |\, 0\,\rangle = 0, \tag{8a}$$

then also [see Eq. (5b)]

$$A_\alpha\, |\, 0\,\rangle = 0, \qquad \text{(for all } \alpha) \tag{8b}$$

The natural definition of N-electron ($N = 2n$) state vector built-up from n geminals is

$$|\, \alpha_1 \alpha_2 \ldots \alpha_n\,\rangle = A_{\alpha_1}^+ A_{\alpha_2}^+ \ldots A_{\alpha_n}^+ \,|\, 0\,\rangle, \tag{9}$$

or

$$\langle\, x_1 x_2 \ldots x_N \,|\, \alpha_1 \alpha_2 \ldots \alpha_n\,\rangle$$

$$= \left(\frac{2^n}{(2n)!}\right)^{1/2} \sum_P (-1)^p P\, \varphi_{\alpha_1}(x_1, x_2) \ldots \varphi_{\alpha_n}(x_{N-1}, x_N), \tag{10}$$

where the summation runs over all $(2n)!/2^n$ permutations of electrons from different geminals, and p is the parity of such permutation P.

The presence of the operator $C_{\alpha\beta}$ in the commutation relations (6) causes serious theoretical and computational difficulties if the operators A_α, A_β^+ are employed as dynamical variables. Especially the states (9) are neither normalized nor orthogonal, and a related difficulty is that Wick's theorem is applicable only to operators satisfying elementary Bose or Fermi commutation or anticommutation rules. To overcome these difficulties, we shall use the method from our recent work[15], where the problem of second-quantization formalism introduced onto a set of nonorthogonal one-particle functions was studied. The

original idea of this approach was initially devised by Dyson in the theory of ferromagnetism[13], and by Girardeau in the second-quantization formalism for a system composed from elementary as well as composite particles[14].

Let us introduce new dynamical-variable operators $\hat{a}_\alpha, \hat{a}_\beta^+$ satisfying elementary Bose commutation rules,

$$[\hat{a}_\alpha, \hat{a}_\beta]_- = 0 = [\hat{a}_\alpha^+, \hat{a}_\beta^+]_-,$$
$$[\hat{a}_\alpha, \hat{a}_\beta^+]_- = \delta_{\alpha\beta}. \tag{11}$$

The corresponding normalized vacuum-state vector should be determined as

$$\hat{a}_\alpha \mid 0) = 0, \qquad \text{(for all } \alpha) \tag{12a}$$

$$(0 \mid 0) = 1. \tag{12b}$$

Following Dyson[13] and Girardeau[14], let us introduce the physical Fock space $\mathscr{F}_P$ as the space of all linear combinations of states (9),

$$\mathscr{F}_P \equiv \{A^+_{\alpha_1} A^+_{\alpha_2} \ldots A^+_{\alpha_n} \mid 0\rangle;\ n \geq 0\}. \tag{13}$$

Similarly, let us introduce the ideal Fock space $\hat{\mathscr{F}}_I$ as the space of all linear combinations of states $\hat{a}^+_{\alpha_1} \hat{a}^+_{\alpha_2} \ldots \mid 0)$,

$$\hat{\mathscr{F}}_I \equiv \{\hat{a}^+_{\alpha_1} \hat{a}^+_{\alpha_2} \ldots \hat{a}^+_{\alpha_n} \mid 0\rangle;\ n \geq 0\}. \tag{14}$$

These spaces can be written as direct sums of orthogonal and noninteracting subspaces,

$$\mathscr{F}_P = \mathscr{F}_P^{(0)} \oplus \mathscr{F}_P^{(1)} \oplus \cdots \oplus \mathscr{F}_P^{(n)} \oplus \cdots, \tag{15a}$$

$$\hat{\mathscr{F}}_I = \hat{\mathscr{F}}_I^{(0)} \oplus \hat{\mathscr{F}}_I^{(1)} \oplus \cdots \oplus \hat{\mathscr{F}}_I^{(n)} \oplus \cdots, \tag{15b}$$

where $\mathscr{F}^{(n)}_{P(I)}$ is a subspace of $\mathscr{F}_{P(I)}$ spanned by states $A^+_{\alpha_1} \ldots A^+_{\alpha_n} \mid 0\rangle$ ($\hat{a}_{\alpha_1} \ldots \hat{a}_{\alpha_n} \mid 0)$) with fixed $n \geq 0$. Between elements of the subspaces $\mathscr{F}_P^{(n)}$ and $\hat{\mathscr{F}}_I^{(n)}$ there is a one-to-one correspondence. Let $\mid \Psi\rangle$ be an element of $\mathscr{F}_P^{(n)}$,

$$\mid \Psi\rangle = \sum_{\alpha_1 \cdots \alpha_n} c(\alpha_1 \ldots \alpha_n) A^+_{\alpha_1} \ldots A^+_{\alpha_n} \mid 0\rangle. \tag{16}$$

In the subspace $\hat{\mathscr{F}}_I^{(n)}$ we can assign to this vector an ideal vector $\mid \Psi)$, or formally $\mid \Psi\rangle \leftrightarrow \mid \Psi)$,

$$\mid \Psi\rangle = \sum_{\alpha_1 \cdots \alpha_n} c(\alpha_1 \ldots \alpha_n) \hat{a}^+_{\alpha_1} \ldots \hat{a}^+_{\alpha_n} \mid 0\rangle, \tag{17}$$

with the same coefficients $C(\alpha_1 \ldots \alpha_n)$ as in (16); and *vice versa*. The purpose of this communication is to demonstrate that the above-introduced map-

ping $\mathscr{F}_P^{(n)} \leftrightarrow \hat{\mathscr{F}}_I^{(n)}$ can be further more deeply specified in the following simple way. Let $|\Psi\rangle, |\Phi\rangle \in \mathscr{F}_P^{(n)}$ and $|\Psi), |\Phi) \in \hat{\mathscr{F}}_I^{(n)}$ be those nonzero vectors for which $|\Psi\rangle \leftrightarrow |\Psi)$ and $|\Phi\rangle \leftrightarrow |\Phi)$. Then, the main conceptual background of the present approach is expressed by these three defining identities

$$\langle \Psi | \Phi \rangle = (\Psi | (1 + \hat{D}) | \Phi), \tag{18}$$

$$\langle \Psi | H | \Phi \rangle = (\Psi | \hat{H} | \Phi), \tag{19}$$

$$\langle \Psi | \Omega_{(p)} | \Phi \rangle = (\Psi | \hat{\Omega}_{(p)} | \Phi), \tag{20}$$

where $(1 + \hat{D})$ is the so called overlap operator, $\hat{H}$ is the so called ideal Hamiltonian, and $\hat{\Omega}_{(p)}$ is the so called ideal observable, corresponding to a p-particle »physical« observable $\Omega_{(p)}$ determined in $\mathscr{F}_P$. The Schrödinger equation determined in the physical Fock space,

$$H | \Psi_i \rangle = E_i | \Psi_i \rangle, \tag{21}$$

is now imagined in ideal Fock space in the ideal Schrödinger equation [see Eqs. (18) and (19)],

$$\hat{H} | \Psi_i) = E_i (1 + \hat{D}) | \Psi_i), \tag{22}$$

where the eigenvectors $|\Psi_i) \in \hat{\mathscr{F}}_I^{(n)}$ are normalized in such a manner that [see Eq. (18)]

$$\langle \Psi_i | \Psi_j \rangle = \delta_{ij} = (\Psi_i | (1 + \hat{D}) | \Psi_j). \tag{23}$$

Then the diagonal and/or nondiagonal matrix elements of an obesrvable $\Omega_{(p)}$ are determined by

$$\langle \Psi_i | \Omega_{(p)} | \Psi_j \rangle = (\Psi_i | \hat{\Omega}_{(p)} | \Psi_j). \tag{24}$$

The ideal Schrödinger equation (22) can be formally rewritten in a form of the standard characteristic problem

$$\hat{H}_{\text{eff}} | \Phi_i) = E_i | \Phi_i), \tag{25}$$

where the Hermitian effective Hamiltonian $\hat{H}_{\text{eff}}$ and its eigenvectors $|\Phi_i)$ are determined by

$$\hat{H}_{\text{eff}} = (1 + \hat{D})^{-1/2} \hat{H} (1 + \hat{D})^{-1/2} \tag{26a}$$

$$|\Phi_i) = (1 + \hat{D})^{1/2} | \Psi_i). \tag{26b}$$

Analogously, the ideal observable $\hat{\Omega}_{(p)}$ from (24) can be also transformed in an effective form,

$$\hat{\Omega}_{(p)\,\text{eff}} = (1 + \hat{D})^{-1/2} \hat{\Omega}_{(p)} (1 + \hat{D})^{-1/2}, \tag{27}$$

where its matrix elements are identical with the l.h.s. of (24),

$$\langle \Psi_i \mid \Omega_{(p)} \mid \Psi_j \rangle = (\Psi_i \mid \hat{\Omega}_{(p),\,\mathrm{eff}} \mid \Psi_j). \tag{28}$$

The ideal effective operators will be studied in the forthcoming three Sections.

The relation (18) is seemingly in contravention with Girardeau's result[14] $\langle \Psi \mid \Phi \rangle = (\Psi \mid \Phi)$. This fact may be simply explained in such a way that an ideal Fock space can be defined by many different approaches, *e. g.* if we define new ideal vectors as $\mid \Psi') = (1 + D)^{1/2} \mid \Psi)$, then we arrive automatically at Girardeau's result $(\Psi' \mid \Phi') = (\Psi \mid (1 + D) \mid \Phi) = \langle \Psi \mid \Phi \rangle$.

3. FEYNMAN-GOLDSTONE DIAMAGNETIC TECHNIQUE

This section deals with the evaluation of the inner product $\langle \alpha_1 \ldots \alpha_n \mid \beta_1 \ldots \beta_n \rangle$ and the matrix elements $\langle \alpha_1 \ldots \alpha_n \mid H \mid \beta_1 \ldots \beta_n \rangle$. In general, these entities can be evaluated directly from their definition applying the commutation rules between the operators A_α, A_β^+ and $\psi(x)$, $\psi^+(y)$. Such an approach is apparently very tedious and rather complex; therefore, in order to facilitate our further theoretical considerations we shall employ a modified version of Feynman-Goldstone diagrammatic technique[16], widely used in all branches of many-body theories[24–26]. Following the expressions (1), (5a-b) and (9), these matrix elements are determined by

$$\langle \alpha_1 \ldots \alpha_n \mid \beta_1 \ldots \beta_n \rangle \tag{29a}$$

$$= \frac{1}{2^n} \int \mathrm{d}V \, \Phi_\alpha^* \langle 0 \mid \psi(x_N) \ldots \psi(x_1) \, \psi^+(x_1') \ldots \psi^+(x_N') \mid 0 \rangle \, \Phi_\beta,$$

$$\langle \alpha_1 \ldots \alpha_n \mid H \mid \beta_1 \ldots \beta_n \rangle \tag{29b}$$

$$= \frac{1}{2^n} \int \mathrm{d}V \, \mathrm{d}x \, \Phi_\alpha^* \langle 0 \mid \psi(x_N) \ldots \psi(x_1) \, \psi^+(x) \, h(x) \, \psi(x) \, \psi^+(x_1') \ldots \psi^+(x_N') \mid 0 \rangle \, \Phi_\beta +$$

$$+ \frac{1}{2^{n+1}} \int \mathrm{d}V \, \mathrm{d}x \, \mathrm{d}y \, \Phi_\alpha^* \langle 0 \mid \psi(x_N) \ldots \psi(x_1) \, \psi^+(x) \, \psi^+(y) \, g(x, y) \, \psi(y) \, \psi(x)$$

$$\psi^+(x_1') \ldots \psi^+(x_N') \mid 0 \rangle \, \Phi_\beta,$$

where $\mathrm{d}V = \mathrm{d}x_1 \ldots \mathrm{d}x_N \, \mathrm{d}x_1' \ldots \mathrm{d}x_N'$, $\Phi_\alpha = \varphi_{\alpha_1}(x_1, x_2) \ldots \varphi_{\alpha_n}(x_{N-1}, x_N)$, and $\Phi_\beta = \varphi_{\beta_1}(x_1', x_2') \ldots (\varphi_{\beta_n}(x_{N-1}', x_N')$. This means that the problem of evaluation of $\langle \alpha_1 \ldots \alpha_n \mid \beta_1 \ldots \beta_n \rangle$ and $\langle \alpha_1 \ldots \alpha_n \mid H \mid \beta_1 \ldots \beta_n \rangle$ is reduced to a calculation of the vacuum-amplitude matrix elements $\langle 0 \mid \psi(x_1) \ldots \psi^+(x_N') \mid 0 \rangle$. With the help of the Feynman-Goldstone diagrammatic technique this problem becomes a mechanical process systematically applicable to all such terms. First of all, we have to introduce the vertices of the present diagrammatic technique, see Figure 1. According to Wick's theorem, the vacuum-amplitude matrix elements are determined by all possible fully contracted terms composed from the products of single elementary contractions $\psi(x) \, \psi^+(x') = \delta(x - x')$. This means that in the present diagrammatic technique there are only the particle lines running from the right to left sides of diagrams. Before proceeding in formulation of the Feynman-Goldstone diagrammatic technique, it is advantageous to introduce some notions and concepts[27] to be used frequently in the following text.

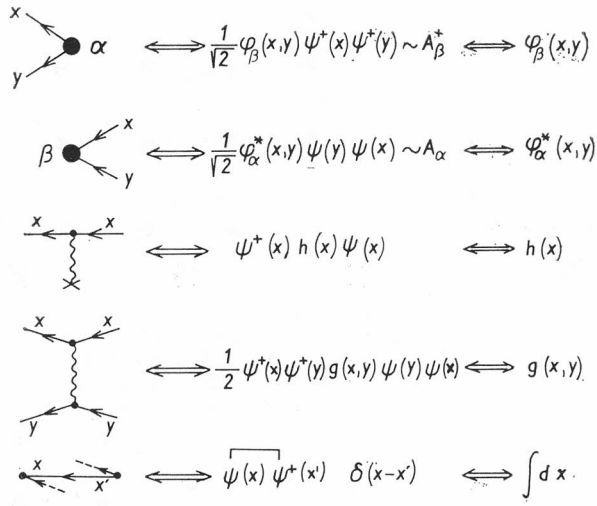

Figure 1. Algebraic interpretation of individual vertices used in the present version of the Feynman-Goldstone diagrammatic technique. The last, fifth, row represents the particle line corresponding to the contraction of electron-field annihilation and creation operator.

A. A diagram which cannot be divided into parts without cutting any particle or interaction line is called *connected,* in the opposite case it is called *disconnected.*

B. A disconnected diagram is made up of connected parts. Each connected part is called a *component.*

C. Two diagrams are *topologically equivalent* if one diagram can be converted into the other by a topological deformation preserving the orientation of lines and the relative positions of vertices, see Figure 2.

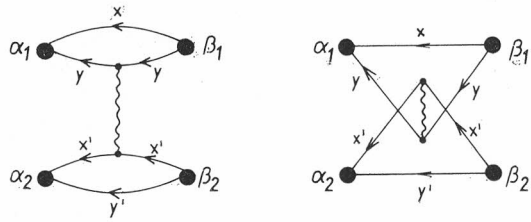

Figure 2. Two topologically equivalent diagrammatic terms (see item C in Section 3).

D. A diagram containing merely the vertices corresponding to the operators A_α, A_β^+ is called *overlap diagram,* see Figure 3, diagram B; in the opposite case, that is, containing a single one- or two-particle vertex, is called *interaction diagram,* see Figure 3, diagrams C and D.

E. Analogously, we define the *overlap component* and the *interaction component.* The *elementary overlap component* is an overlap component built-up from one A_α^- and one A_β^+-vertex, see Figure 4, diagram A. Since we assumed

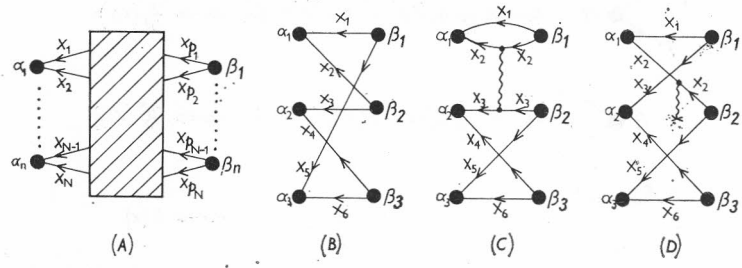

Figure 3. Illustrative examples of possible overlap and interaction diagrammatic terms. Diagram A demonstrates the general diagrammatic term composed of n A_α- and n A_β^+-vertices. Diagram B is the so called overlap diagram, and diagrams C and D are the so called interaction diagrams. Their algebraic interpretation is presented at the end of Section 3.

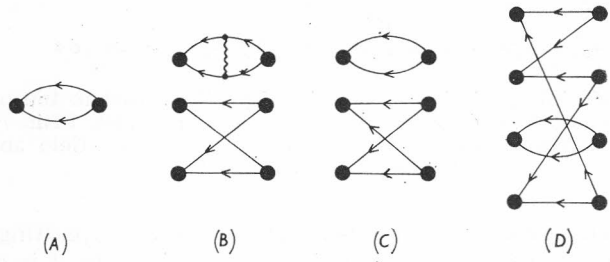

Figure 4. Illustrative examples of different diagrammatic terms and their terminology introduced in Section 3. Diagram A is the elementary overlap component, diagram B is a disconnected but linked interaction term, and diagrams C and D are disconnected unlinked overlap terms.

that the set (3) of geminals forms an orthonormal system, the algebraic interpretation (see below) of this elementary overlap component is $\delta_{\alpha\beta}$. It is easy to see that a disconnected overlap diagram is composed only of (elementary and/or nonelementary) overlap components; a disconnected interaction diagram is composed of one interaction component and one or more overlap components.

F. A diagram that may be generally disconnected or connected, but does not contain an elementary overlap component (see above), is called *linked,* see Figure 4, diagram B; in the opposite case it is called *unliked,* see Figure 4, diagrams C and D. The term »linked« must not be confused with the term »connected«.

G. A set of all topologically nonequivalent overlap (interaction) diagrams made up of $2n$ vertices corresponding to ordered operators, $A_{\alpha_1} \ldots A_{\alpha_n}$ and $A^+_{\beta_1} \ldots A^+_{\beta_n}$ (see Figure 3, diagram A) is denoted $\zeta_0(\alpha_1 \ldots \alpha_n, \beta_1 \ldots \beta_n)$ [$\zeta_I(\alpha_1 \ldots \alpha_n, \beta_1 \ldots \beta_n)$].

Using the above-introduced terminology, the inner product $\langle \alpha_1 \ldots \alpha_n | \beta_1 \ldots \beta_n \rangle$ and the matrix elements $\langle \alpha_1 \ldots \alpha_n | H | \beta_1 \ldots \beta_n \rangle$, both determined by (29), can be expressed in the framework of the Feynman-Goldstone diagrammatic technique by

$$\langle \alpha_1 \ldots \alpha_n | \beta_1 \ldots \beta_n \rangle = \sum_{\Gamma \in \zeta_0(\alpha_1 \ldots \alpha_n, \beta_1 \ldots \beta_n)} \{\Gamma\}, \tag{30a}$$

$$\langle \alpha_1 \dots \alpha_n | H | \beta_1 \dots \beta_n \rangle = \sum_{\Gamma \in \zeta_I (\alpha_1 \dots \alpha_n, \beta_1 \dots \beta_n)} \{\Gamma\}, \tag{30b}$$

where summations run over all diagrammatic terms from the set $\zeta_0 (\alpha_1 \dots \alpha_n, \beta_1 \dots \beta_n)$ and $\zeta_I (\alpha_1 \dots \alpha_n, \beta_1 \dots \beta_n)$, respectively, and $\{\Gamma\}$ denote the »algebraic« interpretation of diagrammatic term Γ. The diagrammatic rules (DRs) establishing a one-to-one correspondence between diagram Γ and its algebraic interpretation $\{\Gamma\}$ are:

DR1: Going from left to right each vertex is assigned its algebraic interpretation; see the third column in Figure 1.

DR2: Each particle line, indexed by an electronic coordinate x, corresponds to an integration $\int dx$. Here we note that a path composed of two particle lines touching an interaction vertex, should be treated as a single particle line; see Figures 2 and 3. This rule directly follows from the fact that one- and two-particle terms of the Hamiltonian (1) are local, that is $\langle x | h | x' \rangle = \delta (x - x') h (x)$ and $\langle xy | g | x'y' \rangle = \delta (x - x') \delta (y - y') g (x, y)$.

DR3: The overall numerical factor is

$$(-1)^p 2^n w, \tag{31}$$

where p is the number of cross points of particle lines, $2n$ is the number of »excitation« vertices (heavy dots), and w is the weight factor determined as the reciprocal value of the number of all automorhisms[28] of the given diagram, including the identical one.

These rules are directly applicable to arbitrarily connected as well as disconnected diagrammatic terms; the algebraic interpretation of a disconnected diagram is simply equal to the product of the algebraic interpretation of its connected components. Formally, suppose a disconnected diagram Γ is composed of components $\Gamma_1, \Gamma_2, \dots$, then $\{\Gamma\} = \{\Gamma_1\}\{\Gamma_2\} \dots$.

Generally, the overall sign of a diagram is determined[29,30] by $(-1)^{h+l+p}$. Here, h and l are the number of internal hole lines and the number of closed loops, respectively, and p is an integer uniquely determined by a proper selection of the phase factor of »external« $2n$-particle states outgoing from the A_β^+-vertices. The diagrammatic terms from (30a-b) are always without hole lines and closed loops, $h = l = 0$; this means that the overall sign is determined only by $(-1)^p$. Integer p may be simply determined as the parity of the permutation

$$\begin{pmatrix} 1 & 2 \dots N \\ p_1 & p_2 \dots p_N \end{pmatrix}$$

where the electronic coordinates $(x_{p_{2i-1}}, x_{p_{2i}})$ are the labels of two particle lines outgoing from A_β^+-vertex indexed by i, for $i = 1, 2, \dots, n$ (see Figure 3, diagram A). Finally, the parity p (its eveness or oddness) is equivalent to the number of the cross points of particle lines, which has been demonstrated.

A similar simple consideration as just above leads to the numerical factor $2^n w$ from (31). For instance, let us consider a diagram from the r.h.s of (29a). Each A_α^- and A_β^+-vertex can be contracted with the rest of diagram in two

fully equivalent ways; that is for the given overlap (and also for an interaction diagram with one-particle vertex) we have $2^{2n}\,w$ distinct contractions leading to the same diagram. Here, w is the number (weight factor[28]) ensuring that each distinct contraction should be included once and only once. When the given diagram has some topological symmetry (formally treated through the concept of topological automorphisms[28]), some contractions from all 2^{2n} ways cannot be considered as distinct; this is avoided by dividing them by an appropriate number $1/w$. Therefore, multiplying $2^{2n}\,w$ by factor 2^{-n} from the front of (29a), we obtain the same result as in (31).

For illustration, we are presenting the algebraic interpretation of diagrams B, C, and D in Figure 3.

Diagram B: $n = 3$, $w = 1$, and $p = 3$,

$$-8 \int \mathrm{d}V\, \varphi^{*}_{\alpha_1}(x_1, x_2)\, \varphi^{*}_{\alpha_2}(x_3, x_4)\, \varphi^{*}_{\alpha_3}(x_5', x_6')\, \varphi_{\beta_1}(x_1', x_5')\, \varphi_{\beta_2}(x_2', x_3')\, \varphi_{\beta_3}(x_4', x_6').$$

Diagram C: $n = 3$, $w = 1$, and $p = 1$,

$$-8 \int \mathrm{d}V\, \varphi^{*}_{\alpha_1}(x_1, x_2)\, \varphi^{*}_{\alpha_2}(x_3, x_4)\, \varphi^{*}_{\alpha_3}(x_5, x_6)\, g(x_2, x_3)\, \varphi_{\beta_1}(x_1, x_2)\, \varphi_{\beta_3}(x_3, x_5)\, \varphi_{\beta_2}(x_4, x_6).$$

Diagram D: $n = 3$, $w = 1$, and $p = 2$,

$$+8 \int \mathrm{d}V\, \varphi^{*}_{\alpha_1}(x_1, x_2)\, \varphi^{*}_{\alpha_2}(x_3, x_4)\, \varphi^{*}_{\alpha_3}(x_5, x_6)\, h(x_2)\, \varphi_{\beta_1}(x_1, x_3)\, \varphi_{\beta_2}(x_2, x_5)\, \varphi_{\beta_3}(x_4, x_6).$$

4. OVERLAP OPERATOR

The overlap operator defined by (9) will be now constructed in terms of the ideal operators $\hat{a}_\alpha$ and $\hat{a}^{+}_\beta$. Let $A(i_1 \ldots i_t,\ j_1 \ldots j_t)$ be determined as the sum of all linked overlap diagrammatic terms from the set $\zeta_{0,\mathrm{L}}(i_1, \ldots, i_t, j_1, \ldots, j_t) \subset \subset \zeta_0(i_1, \ldots, i_t, j_1, \ldots, j_t)$, where $\zeta_{0,\mathrm{L}}(i_1, \ldots, i_t, j_1, \ldots, j_t)$ denotes a subset $\zeta_0(i_1, \ldots, i_t, j_1, \ldots, j_t)$ containing merely the linked diagrams (see Figure 5),

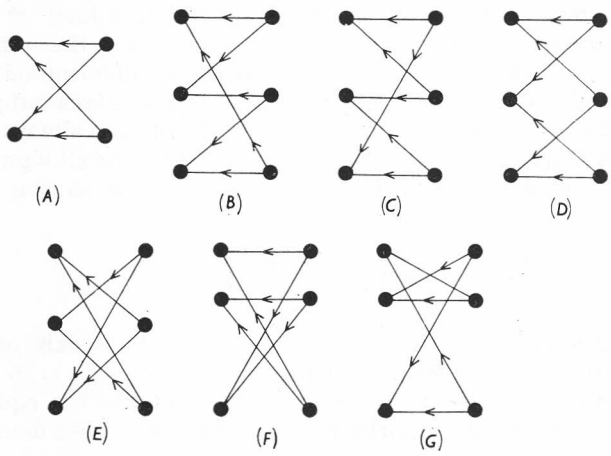

Figure 5. The overlap linked diagrammatic terms contributing to the matrix elements $A(i_1 \ldots i_t, j_1 \ldots j_t)$ determined by Eq. (32). In particular, diagram A contributes to $A(i_1\, i_2, j_1\, j_2)$, and diagrams B—G contribute to $A(i_1\, i_2\, i_3, j_1\, j_2\, j_3)$.

$$A(i_1 \ldots i_t, j_1 \ldots j_t) = \sum_{\Gamma \in \zeta_{0,L}(i_1 \ldots i_t,\, j_1 \ldots j_t)} \{\Gamma\}, \tag{32}$$

for $t \geq 2$; for $t = 1$ there are no linked overlap diagrams, the subset $\zeta_0(i_1, j_1)$ contains only one elementary component. We next symmetrize the $A(i_1, \ldots, i_t, j_1, \ldots, j_t)$'s,

$$\langle i_1 \ldots i_t \,||\, j_1 \ldots j_t \rangle_L = \sum_P A(i_{p_1} \ldots i_{p_t}, j_{p_1} \ldots j_{p_t}), \tag{33}$$

where summation runs over all permutations

$$P = \begin{pmatrix} 1 & 2 \ldots t \\ p_1 & p_2 \ldots p_t \end{pmatrix} \tag{34}$$

and the subscript L denotes that only linked (generally connected or disconnected) diagrammatic terms are taken into account. Using these overlap matrix elements (33) we define the following operator as

$$\hat{D}_L^{(t)} = \frac{1}{t!} \sum_{\substack{i_1 \ldots i_t \\ j_1 \ldots j_t}} \langle i_1 \ldots i_t \,||\, j_1 \ldots j_t \rangle_L \hat{a}^+_{i_1} \ldots \hat{a}^+_{i_t} \hat{a}^+_{j_t} \ldots \hat{a}_{j_1}, \tag{35a}$$

$$(\hat{D}_L^{(t)})^+ = \hat{D}_L^{(t)}. \tag{35b}$$

Finally, the overlap operator from (18) can be then determined as

$$1 + \hat{D} = 1 + \sum_{t \geq 2} \hat{D}_L^{(t)} \tag{36}$$

$$= 1 + \sum_{t \geq 2} \frac{1}{t!} \sum_{\substack{i_1 \ldots i_t \\ j_1 \ldots j_t}} \langle i_1 \ldots i_t \,||\, j_1 \ldots j_t \rangle_L \hat{a}_{i_1} \ldots \hat{a}^+_{i_t} \hat{a}_{j_t} \ldots \hat{a}^+_{j_1},$$

where

$$\begin{aligned} \langle \alpha_1 \ldots \alpha_n \,|\, \beta_1 \ldots \beta_n \rangle &= (\alpha_1 \ldots \alpha_n \,|\, (1 + \hat{D}) \,|\, \beta_1 \ldots \beta_n) \\ &= (\alpha_1 \ldots \alpha_n \,|\, \beta_1 \ldots \beta_n) + \sum_{t=2}^{n} (\alpha_1 \ldots \alpha_n \,|\, \hat{D}_L^{(t)} \,|\, \beta_1 \ldots \beta_n), \end{aligned} \tag{37}$$

since $(\alpha_1 \ldots \alpha_n \,|\, \hat{D}_L^{(t)} \,|\, \beta_1 \ldots \beta_n) = 0$ for $t > n$. The states $|\, \alpha_1 \ldots \alpha_n)$, $|\, \beta_1 \ldots \beta_n)$, are taken from $\hat{\mathscr{F}}_I^{(n)}$ and they are determined as $|\, \alpha_1 \ldots \alpha_n) = \hat{a}^+_{\alpha_1} \ldots \hat{a}^+_{\alpha_n} |\, 0)$ and $|\, \beta_1 \ldots \beta_n) = \hat{a}^+_{\beta_1} \ldots \hat{a}^+_{\beta_n} |\, 0)$. The first row of (37) immediately gives the general defining expression (18) of the overlap operator $(1 + \hat{D})$. The term $(\alpha_1 \ldots \alpha_n |$ $|\, \beta_1 \ldots \beta_n)$ determines those overlap diagrammatic terms of $\langle \alpha_1 \ldots \alpha_n \,|\, \beta_1 \ldots \beta_n \rangle$ [see Eq. (30a)] which are composed of n elementary overlap components. The term $(\alpha_1 \ldots \alpha_n \,|\, \hat{D}_L^{(t)} \,|\, \beta_1 \ldots \beta_n)$ determines those terms of $\langle \alpha_1 \ldots \alpha_n \,|\, \beta_1 \ldots \beta_n \rangle$ which (1) are composed of $(n - t)$ elementary overlap components, and

(2) the remaining part (generally connected or disconnected) of the diagram contains only linked overlap components.

Similar considerations point to the conclusion that each operator $\hat{D}_L^{(t)}$ can be uniquely divided into two parts,

$$\hat{D}_L^{(t)} = \hat{D}_{L,C}^{(t)} + \hat{D}_{L,DC}^{(t)} \tag{38}$$

where $\hat{D}_{L,C}^{(t)}$ ($\hat{D}_{L,DC}$) denotes the part of $\hat{D}_L^{(t)}$ which contains only linked connected (linked disconnected) diagrammatic terms. In particular, operators $\hat{D}_L^{(2)}$ and $\hat{D}_L^{(3)}$ have only the connected part; their disconnected part should be zero. The disconnected parts can be formed only from two or more elementary components producing the diagrams of unlinked nature. The disconnected part of $\hat{D}_L^{(4)}$ can be produced, formally, as a normal product of two »connected« operators $\hat{D}_{L,C}^{(2)}$,

$$\hat{D}_{L,DC}^{(4)} = \frac{1}{2!} N [\hat{D}_{L,C}^{(2)} \hat{D}_{L,C}^{(2)}], \tag{39}$$

where $N[\ldots]$ denotes the normal product[23,24] of the ideal creation and annihilation operators. Let $A_1, A_2, A_3, \ldots$ denote arbitrary creation and/or annihilation operators $\hat{a}_\alpha^+, \hat{a}_\beta$. Then the present normal product, defined with respect to the vacuum state $|0)$, is determined by $N[A_1 A_2 A_3 \ldots] = A_{p_1} A_{p_2} A_{p_3} \ldots$. Here $A_{p_1} A_{p_2} A_{p_3} \ldots$ is any permutation of the original product $A_1 A_2 A_3 \ldots$ which are rearranged in such a manner that, reading from right to left, first come all annihilation operators and then all creation operators. For instance $N[\hat{a}_l^+ \hat{a}_k \hat{a}_{k'} \hat{a}_{l'}^+] = \hat{a}_l^+ \hat{a}_{l'}^+ \hat{a}_k \hat{a}_{k'}$. The numerical factor 1/2!, standing in front of (39), was introduced since this procedure produces two topologically equivalent disconnected diagrams with the same algebraic interpretation. Generally, the operator $\hat{D}_L^{(t)}$ for $(t \geqslant 2)$ can be determined as

$$\hat{D}_L^{(t)} = \sum_{n_2, n_3, \ldots} \frac{1}{n_2! n_3! \ldots} N [(\hat{D}_{L,C}^{(2)})^{n_2} (\hat{D}_{L,C}^{(3)})^{n_3} \ldots], \tag{40}$$

where the nonnegative integers $n_2, n_3, \ldots$ are constrained by

$$2n_2 + 3n_3 + \ldots = t. \tag{41}$$

This means that the overlap operator $(1 + \hat{D})$ can formally be written in the following compact form:

$$1 + \hat{D} = N [\exp (\hat{D}_{L,C})], \tag{42a}$$

$$\hat{D}_{L,C} = \sum_{t \geqslant 2} \hat{D}_{L,C}^{(t)}. \tag{42b}$$

This result represents a formal counterpart of the well-known »linked-cluster« theorems from Iwamoto-Yamada model of nuclear systems[17–21].

5. MODEL HAMILTONIAN

The basic idea is now to establish a one-to-one correspondence between the matrix elements $\langle\, \alpha_1 \dots \alpha_n \,|\, H \,|\, \beta_1 \dots \beta_n \,\rangle$ and $(\alpha_1 \dots \alpha_n \,|\, \hat{H} \,|\, \beta_1 \dots \beta_n)$ in the sense of defining relation (19). We have to construct an ideal Hamiltonian $\hat{H}$, defined in the ideal Fock space $\hat{\mathscr{F}}_{\mathrm{I}}$, in such a manner that

$$\langle \alpha_1 \dots \alpha_n \,|\, H \,|\, \beta_1 \dots \beta_n \,\rangle = (\alpha_1 \dots \alpha_n \,|\, \hat{H} \,|\, \beta_1 \dots \beta_n). \tag{43}$$

Let $B\,(i_1 \dots i_t, j_1 \dots j_t)$ be determined as the sum of all linked interaction diagrammatic terms from the set $\zeta_{\mathrm{I,L}}\,(i_1 \dots i_t, j_1 \dots j_t) \subset \zeta_{\mathrm{I}}\,(i_1 \dots i_t, j_1 \dots j_t)$, where $\zeta_{\mathrm{I,L}}\,(i_1 \dots i_t, j_1 \dots j_t)$ denotes a subset of $\zeta_{\mathrm{I}}\,(i_1 \dots i_t, j_1 \dots j_t)$ containing merely the linked diagrams (see Figure 6),

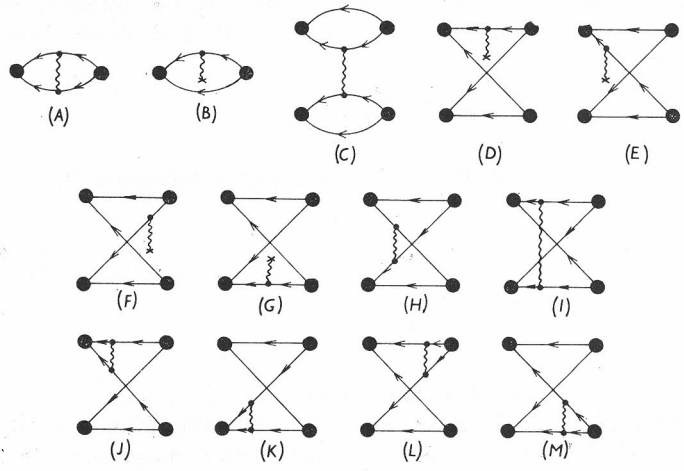

Figure 6. The interaction linked diagrammatic terms contributing to the matrix elements $B\,(i_1 \dots i_t, j_1 \dots j_t)$ determined by Eq. (44). In particular, diagrams A and B contribute to $B\,(i_1, j_1)$, and diagrams C—M contribute to $B\,(i_1\, i_2, j_1\, j_2)$.

$$B\,(i_1 \dots i_t, j_1 \dots j_t) = \sum_{\Gamma \in \zeta_{\mathrm{I,L}}\,(i_1 \dots i_t,\, j_1 \dots j_t)} \{\Gamma\}, \tag{44}$$

for $t \geqslant 1$. We next symmetrize the $B\,(i_1 \dots i_t, j_1 \dots j_t)$'s,

$$\{i_1 \dots i_t, j_1 \dots j_t\}_{\mathrm{L}} = \sum_{P} B\,(i_{\mathrm{p}_1} \dots i_{\mathrm{p}_t}, j_{\mathrm{p}_1} \dots j_{\mathrm{p}_t}), \tag{45}$$

where summation runs over all permutation P determined by (34), and the subscript L means that only linked (generally connected or disconnected) diagrammatic terms were taken into account. Using these »interaction« matrix elements (45), let us define

$$\hat{H}_{\mathrm{L}}^{(t)} = \frac{1}{t!} \sum_{\substack{i_1 \dots i_t \\ j_1 \dots j_t}} \{i_1 \dots i_t \,||\, j_1 \dots j_t\}_{\mathrm{L}}\, \hat{a}^{+}_{i_1} \dots \hat{a}^{+}_{i_t}\, \hat{a}_{j_t} \dots \hat{a}_{j_1}, \tag{46a}$$

$$(\hat{H}_{\mathrm{L}}^{(t)})^{+} = \hat{H}_{\mathrm{L}}^{(t)}. \tag{46b}$$

Finally, the ideal Hamiltonian $\hat{H}$ from (43) can then be determined as

$$\hat{H} = \sum_{t \geqslant 1} \hat{H}_{\mathrm{L}}^{(t)}, \tag{47}$$

where

$$\begin{aligned} \langle \alpha_1 \ldots \alpha_n | H | \beta_1 \ldots \beta_n \rangle &= (\alpha_1 \ldots \alpha_n | \hat{H} | \beta_1 \ldots \beta_n) \\ &= \sum_{t=1}^{n} (\alpha_1 \ldots \alpha_n | \hat{H}^{(t)} | \beta_1 \ldots \beta_n), \end{aligned} \tag{48}$$

since $(\alpha_1 \ldots \alpha_n | \hat{H}_{\mathrm{L}}^{(t)} | \beta_1 \ldots \beta_n) = 0$ for $t > n$.

The diagrammatic contributions from (44) may be uniquely divided onto two disjoint subsets, those linked and connected, and those linked and disconnected, then

$$\hat{H} = \hat{H}_{\mathrm{L,C}} + \hat{H}_{\mathrm{L,CD}}. \tag{49}$$

The connected part $\hat{H}_{\mathrm{L,C}}$ of $\hat{H}$ can be formally determined in the same way as (47),

$$\hat{H}_{\mathrm{L,C}} = \sum_{t \geq 1} \hat{H}_{\mathrm{L,C}}^{(t)} = \sum_{t \geq 1} \frac{1}{t!} \sum_{\substack{i_1 \ldots i_t \\ j_1 \ldots j_t}} \{ i_1 \ldots i_t \,||\, j_1 \ldots j_t \}_{\mathrm{L,C}} \hat{a}_{i_1}^{+} \ldots \hat{a}_{i_t}^{+} \hat{a}_{j_t} \ldots \hat{a}_{j_1}. \tag{50}$$

Here, the symmetric matrix elements $\{ i_1 \ldots i_t \,||\, j_1 \ldots j_t \}_{\mathrm{L,C}}$ are defined analogously as $\{ i_1 \ldots i_t \,||\, j_1 \ldots j_t \}_{\mathrm{L}}$ [see Eqs. (44) and (45)]. Now the summation in (44) runs over all linked and connected interaction diagrammatic terms from $\zeta_{\mathrm{I,L}}(i_1 \ldots i_t, j_1 \ldots j_t)$. The disconnected part $\hat{H}_{\mathrm{L,DC}}$ of $\hat{H}$ is built-up from the linked and disconnected diagrammatic terms from (44); they contain one interaction component and one or more overlap components. Since the disconnected parts of the operators $\hat{H}_{\mathrm{L}}^{(t)}$, defined by (46a), cannot be composed of the elementary overlap components [the pertinent diagrammatic terms from (44) are linked], we have

$$\hat{H}_{\mathrm{L}}^{(t)} = \hat{H}_{\mathrm{L,C}}^{(t)}, \qquad (\text{for } t = 1, 2), \tag{51}$$

that is, their disconnected parts should automatically be zero. But the next operators $\hat{H}_{\mathrm{L}}^{(t)}$, for $t \geqslant 3$, can already be decomposed on disconnected, as well as the connected part. The connected part is identical with the operator $\hat{H}_{\mathrm{L,C}}^{(t)}$ defined by (50), and their disconnected part can formally be evaluated in a way analogous to (39) and (40). For instance,

$$\hat{H}_{\mathrm{L}}^{(3)} = \hat{H}_{\mathrm{L,C}}^{(3)} + N [\hat{H}_{\mathrm{L,C}}^{(1)} \hat{D}_{\mathrm{L,C}}^{(2)}], \tag{52a}$$

$$\hat{H}^{(4)}_{L} = \hat{H}^{(4)}_{L,C} + N\,[\hat{H}^{(2)}_{L,C}\,\hat{D}^{(2)}_{L,C}] + N\,[\hat{H}^{(3)}_{L,C}\,\hat{D}^{(3)}_{L,C}], \tag{52b}$$

$$\hat{H}^{(5)}_{L} = \hat{H}^{(5)}_{L,C} + N\,[\hat{H}^{(2)}_{L,C}\,\hat{D}^{(3)}_{L,C}] + N\,[\hat{H}^{(3)}_{L,C}\,\hat{D}^{(2)}_{L,C}] + \frac{1}{2!}N\,[\hat{H}^{(1)}_{L,C}\,\hat{D}^{(2)}_{L,C}\,\hat{D}^{(2)}_{L,C}], \tag{52c}$$

Generally, the disconnected part $\hat{H}_{L,DC}$ of the full ideal Hamiltonian $\hat{H}$ [see Eq. (49)] can be determined as follows:

$$\hat{H}_{L,DC} = N\,[\hat{H}_{L,C}\,\hat{D}], \tag{53}$$

where the operator $\hat{D}$ is defined by (36) or (42). Introducing (53) into (49) and using (42), we obtain the final form of the ideal Hamiltonian expressed through the linked-connected diagrammatic terms,

$$\hat{H} = N\,[\hat{H}_{L,C}\,(1 + \hat{D})] = N\,[\hat{H}_{L,C}\exp(\hat{D}_{L,C})], \tag{54}$$

where the following three simple properties of the normal product have been used: $N\,[\hat{H}_{L,C}] = \hat{H}_{L,C}$, $N\,[\hat{X} + \hat{Y}] = N\,[\hat{X}] + N\,[\hat{Y}]$, and $N\,[\hat{X}N\,[\hat{Y}]] = N\,[\hat{X}\hat{Y}]$, for arbitrary ideal operators X and Y. The result (54) is nothing else than a form of the »linked-cluster« theorem realized for the present ideal Hamiltonian. According to result (54), the ideal Hamiltonian can be written in a form quite similar to that recently considered by Schrieffer[31] and Kvasnička[15] in the second-quantization formalism introduced on a set of nonorthogonal one-particle functions,

$$\hat{H} = \sum_{t \geqslant 1} \hat{H}^{(t)}, \tag{55a}$$

$$\hat{H}^{(t)} = \frac{1}{t!} \sum_{\substack{i_1 \ldots i_t \\ j_1 \ldots j_t}} \{i_1 \ldots i_t \,\|\, j_1 \ldots j_t\}_{L,C}\, \hat{a}^{+}_{i_1} \ldots \hat{a}^{+}_{i_t}\,(1 + D)\,\hat{a}_{j_t} \ldots \hat{a}_{j_1}. \tag{55b}$$

The symmetrical matrix elements $\{i_1 \ldots i_t \,\|\, j_1 \ldots j_t\}_L$ from (47) are expressed in terms of the interaction and overlap linked-connected matrix elements [*cf.* Eqs. (51) and (52)],

$$\{i_1 \,\|\, j_1\}_L = \{i_1 \,\|\, j_1\}_{L,C}, \tag{56a}$$

$$\{i_1 i_2 \,\|\, j_1 j_2\}_L = \{i_1 i_2 \,\|\, j_1 j_2\}_{L,C}, \tag{56b}$$

$$\{i_1 i_2 i_3 \,\|\, j_1 j_2 j_3\}_L = \{i_1 \,\|\, j_1\}_{L,C} \langle i_2 i_3 \,\|\, j_2 j_3 \rangle + \{i_2 \,\|\, j_2\} \langle i_1 i_3 \,\|\, j_1 j_3 \rangle_{L,C} + \{i_3 \,\|\, j_3\} \langle i_1 i_2 \,\|\, j_1 j_2 \rangle_{L,C}, \tag{56c}$$

and quite analogously for subsequent matrix elements $\{i_1 \ldots i_t \,\|\, j_1 \ldots j_t\}_L$, $t \geq 4$.

5.1. Effective Hamiltonian

Let us now turn our attention to the construction of the effective Hamiltonian $\hat{H}_{eff}$ defined by (26a). Since the set (3) is formed from linearly independent two-particle functions, the existence of this operator is ensured by

the fact that the overlap operator $(1 + \hat{D})$ should be a positively definite operator. Moreover, assuming[32] that all eigenvalues of the overlap operator are less than one, then the operator $(1 + \hat{D})^{-1/2}$ can be expressed as

$$(1 + \hat{D})^{-1/2} = \sum_{m=0}^{\infty} \binom{-1/2}{m} \hat{D}^{vt} = 1 - \frac{1}{2}\hat{D} + \frac{3}{8}\hat{D}^2 \ldots . \tag{58}$$

Introduction of (58) into (26a) gives

$$\hat{H}_{\text{eff}} = \hat{H} - \frac{1}{2}[\hat{H}, \hat{D}]_+ + \frac{3}{8}[[\hat{H}, \hat{D}]_+, \hat{D}]_+ - \frac{1}{2}\hat{D}\hat{H}\hat{D}\hat{D} + \ldots . \tag{59}$$

Using the commutation relations (11), this effective Hamiltonian has the following form similar to (47),

$$\hat{H}_{\text{eff}} = \sum_{t \geqslant 1} \hat{H}^{(t)}_{\text{eff}}, \tag{60a}$$

$$\hat{H}^{(t)}_{\text{eff}} = \frac{1}{t!} \sum_{\substack{i_1 \ldots i_t \\ j_1 \ldots j_t}} \{i_1 \ldots i_t \,\|\, j_1 \ldots j_t\}_{\text{eff}} \hat{a}^+_{i_1} \ldots \hat{a}^+_{i_t} \hat{a}_{j_t} \ldots \hat{a}_{j_1}, \tag{60b}$$

where the matrix elements $\{i_1 \ldots i_t \,\|\, j_1 \ldots j_t\}_{\text{eff}}$ should be symmetric with respect to an arbitrary permutation of indices $(i_1 \ldots i_t)$ and $(j_1 \ldots j_t)$,

$$\{i_1 \ldots i_t \,\|\, j_1 \ldots j_t\}_{\text{eff}} = \{i_{p_1} \ldots i_{p_t} \,\|\, j_{p_1} \ldots j_{p_t}\}_{\text{eff}}. \tag{61}$$

Unfortunately, it is probably impossible to construct a counterpart of the »linked-cluster« theorem similar to (54) or (42) for the effective Hamiltonian.

6. IDEAL OBSERVABLE

In this Section the methods developed in the previous Section 5 are applied to the construction of an ideal observable defined by (20). Since the used theoretical considerations and algebraic manipulations are formally very similar to those from Section 5, only a brief outline of the neccessary theory is given here.

The p-particle observable $\Omega_{(p)}$ in the second-quantization formalism [23] is determined by

$$\Omega_{(p)} = \frac{1}{p!} \int dx_1 \ldots dx_p \, \psi^+(x_1) \ldots \psi^+(x_p) \, \omega(x_1, \ldots, x_p) \, \psi(x_p) \ldots \psi(x_1), \tag{62}$$

where $\omega(x_1, \ldots, x_p)$ is a symmetric Hermitian operator acting on the variable $x_1, \ldots, x_p$. First of all we have to introduce the diagrammatic interpretation of the p-particle observable $\Omega_{(p)}$, that is we assign to the operator $\omega(x_1, \ldots, x_p)$ a vertex composed from p outgoing and incoming particle lines. Then, the basic relations (30a-b) can be completed by

$$\langle \alpha_1 \ldots \alpha_n \,|\, \Omega_{(p)} \,|\, \beta_1 \ldots \beta_n \rangle = \sum_{\Gamma \in \xi_{\text{OBS}}(\alpha_1 \ldots \alpha_n, \beta_1 \ldots \beta_n)} \{\Gamma\}, \tag{63}$$

where the summation runs over all diagrammatic terms Γ from the set

$\zeta_{\mathrm{OBS}}(\alpha_1 \ldots \alpha_n, \beta_1 \ldots \beta_n)$ formed from all topologically nonequivalent observable diagrams. Giving the same arguments as in Section 5, the ideal observable $\hat{\Omega}_{(p)}$ can be determined by the following »linked-cluster« theorem

$$\hat{\Omega}_{(p)} = N\,[\hat{\Omega}_{(p)\,\mathrm{L,C}} \exp(\hat{D}_{\mathrm{L,C}})], \tag{64}$$

where $\hat{\Omega}_{(p)\,\mathrm{L,C}}$ is that part of the full ideal observable $\hat{\Omega}_{(p)}$ which is composed merely of linked and disconnected observable diagrammatic terms,

$$\hat{\Omega}_{(p)\,\mathrm{L,C}} = \sum_{t \geqslant p-1} \hat{\Omega}^{(t)}_{(p)\,\mathrm{L,C}} \tag{65a}$$

$$\hat{\Omega}^{(t)}_{(p)\,\mathrm{L,C}} = \frac{1}{t!} \sum_{\substack{i_1 \ldots i_t \\ j_1 \ldots j_t}} [i_1 \ldots i_t \,\|\, j_1 \ldots j_t]_{\mathrm{L,C}}\, \hat{a}^{+}_{i_1} \ldots \hat{a}^{+}_{i_t}\, \hat{a}_{j_1} \ldots \hat{a}_{j_t}. \tag{65b}$$

Here, the symmetrized matrix elements $[i_1 \ldots i_t \,\|\, j_1 \ldots j_t]_{\mathrm{L,C}}$ [*cf.* Eq. (50)] are evaluated on the basis of all linked-connected diagrammatic terms belonging to the set $\zeta_{\mathrm{OBS}}(i_1 \ldots i_t, j_1 \ldots j_t)$. Similarly as in (55a-b) this ideal operator can be written as follows:

$$\hat{\Omega}_{(p)} = \sum_{t \geqslant p-1} \hat{\Omega}^{(t)}_{(p)}, \tag{66a}$$

$$\hat{\Omega}^{(t)}_{(p)} = \frac{1}{t!} \sum_{\substack{i_1 \ldots i_t \\ j_1 \ldots j_t}} [i_1 \ldots i_t \,\|\, j_1 \ldots j_t]_{\mathrm{L,C}}\, a^{+}_{i_1} \ldots \hat{a}^{+}_{i_t} (1 + \hat{D})\, \hat{a}_{j_1} \ldots \hat{a}_{j_t}. \tag{66b}$$

The effective form of the ideal observable, $\hat{\Omega}_{(p),\,\mathrm{eff}}$, is constructed by a method similar to the effective Hamiltonian, so we shall not repeat it here.

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SAŽETAK

Formalizam druge kvantizacije za spregnute antisimetrične dvočestične valne funkcije (geminals)

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Opisana je metoda konstrukcije formalizma druge kvantizacije na skupu ortogonalnih geminala (antisimetričnih dvočestičnih valnih funkcija). U tu svrhu upotrijebljeni su tzv. idealni operatori stvaranja i poništenja čestica koji zadovoljavaju Boseova komutacijska pravila. Pokazano je da se hamiltonijan kao i ostale opservable mogu jednoznačno izraziti s pomoću uvedenih idealnih operatora. Da bi se olakšalo računanje ovih posljednjih, upotrijebljena je modificirana verzija Feynman-Goldstonove dijagramske tehnike.