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Extended coupled-cluster method. I. Generalized coherent bosonization as a mapping of quantum theory into classical Hamiltonian mechanics

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The quantum-mechanical many-body problem is studied using the extended coupled-cluster method (ECCM) as a convenient parametrization of the Hilbert space. A systematic development of the formalism is given, and the quantum-mechanical problem is cast into the form of a classical Hamiltonian field theory in a complex symplectic phase space. The equations of motion of the basic ECCM amplitudes are derived both from a dynamical action principle using the ECCM average-value functional, and directly from the Schrödinger equation using the ECCM double similarity transformation. Rules are given for the construction of the Hamiltonian and other observables as well as their products. In particular, commutators are shown to be mapped into generalized classical Poisson brackets. The description is interpreted as an exact bosonization of the quantum theory in which the concept of bosonization is carried to the logical extreme, namely, the resulting generalized coherent bosons are identifiable with classical fields. The quantum-mechanical states of the system are points in the ECCM phase space, and their time evolution, or trajectories, are controlled by a classical Hamiltonian. The bosonization has a perturbation-theoretical basis in terms of maximally linked generalized tree diagrams. The increased degree of locality of the basic amplitudes allows applications to topological excitations and cases with spontaneous symmetry breaking.

I. INTRODUCTION

The ground state of an interacting many-body system can be parametrized by an exponential operator ($\exp S$) acting on the noninteracting model state.[1] The perturbation expansion of the operator S is composed of linked terms only, and the $\exp S$ representation for the ground state is conceptually comparable to the cumulant expansions in many other problems of probabilistic nature. Coester[2] and Kümmel[3] introduced a similarity transformation using the linked-cluster operator S as the generator, and laid down the basis for the theory which since then has been known as the $\exp S$ or coupled-cluster method (CCM).[2-6] By now, the number of applications of the method has become very large and they cover a wide variety of physical problems, for example, in nuclear physics,[4,6] quantum chemistry,[5,7-10] theory of homogeneous electron liquid,[11-13] and, more recently, in relativistic field theory.[14-16]

The essence of CCM, as contrasted against, e.g., the configuration-interaction (CI) method,[17] is in the increased degree of locality in the description of many-body correlation phenomena. The CI method contains unlinked diagrams for the energy and suffers accordingly from the size-extensivity problem,[6,18,19] which difficulty is resolved in the CCM description. Together with the generalized time-ordering (GTO) properties of the associated generalized tree diagrams these features have proven to be highly useful not only for large systems but also for systems with only a small number of degrees of freedom.[4,6,20,21] Various theoretical extensions of the conventional CCM have been introduced, e.g., for the purposes of degenerate-perturbation theory,[22,8] excited states and excitation energies,[21-23] and treatment of sum rules.[24,25] The method was also generalized into a full dynamical theory for time-dependent properties by allowing the CCM amplitudes S to depend on time and imposing the time-dependent Schrödinger equation.[26]

The evaluation of average values of observables other than the energy makes it necessary to parametrize also the bra ground state. This can be done in several ways. The most straightforward method is to use the $\exp S$ ansatz also for the bra state, but with the operator $S^{\dagger}$, and to admit for the average value of the observable only the connected diagrams.[27] This method as well as the more advanced methods of Lührmann[28] or Kümmel[28] are in truncated approximations in conflict with the Feynman-Hellman theorem, which requires the diagrams for the average value of an observable to be obtained from those for the energy by replacing each Hamiltonian vertex in turn by the observable in question.[29] Subsequently, Monkhorst gave a novel formulation for the computa-

tion of average values compatible with the Feynman-Hellman requirement, without, however, introducing an explicit average-value functional.[26]

It was later shown by one of the present authors[30] that it is possible to introduce various parametrizations for the bra state which are not only compatible with the Feynman-Hellman theorem, but which also allow the new amplitudes characterizing the bra state (Ω or S'') as well as the old amplitudes S to be obtained from a variational principle. The "normal CCM" with its parameters Ω is a straightforward generalization of Monkhorst's method.[26] Corresponding to the ground state of the system, the operator Ω was shown to be composed of unlinked terms and to be expressible in the form $\Omega=\exp(S'')$, where the new amplitudes S'' are linked.[30] By considering the amplitudes S'' to be independent basic variables one then obtains a method which originally was called the "extended exp$S$ method,"[30] but which we now prefer to call the "extended coupled-cluster method" or ECCM (this term should not be confused with a similar one used in some quantum chemistry papers to indicate an approximation beyond the singles and doubles, i.e., beyond the SUB2 truncation level).

The ECCM parametrization is based on a double similarity transformation rather than a single one, and it can be shown to lead to a GTO property both forwards and backwards in time for the corresponding doubly linked generalized tree diagrams, as far as the ground-state energy is concerned.[30] The method was also generalized to time-dependent phenomena[30] using a dynamical variational principle, and to excited states[30,31] through the linearization of small oscillations around the ground state. The method was shown to agree at its lowest truncation level with the mean-field theory or the semiclassical approximation, which makes it applicable to cases where, e.g., spontaneous symmetry breaking may occur.[30–32] Comparisons of ECCM at low truncation levels with other prescriptions for average values have been done by Pal, who also applied ECCM to a study of higher-order static-response properties.[33]

In view of the above properties the present paper is dedicated to a systematic development of the general formalism of the extended coupled-cluster method. The basic mathematical objects in this method are subsystem amplitudes or linked configuration excitation amplitudes, and therefore we begin in Sec. II with a brief description of general many-body operator algebra in a Hilbert space. It will be useful to introduce an effective shorthand notation for the operators and the amplitudes, and a notation for compounding the many-body configuration indices. In Sec. III we give a description of the basic ECCM amplitudes and the general structure of the average-value functional. Section IV derives connections between the matrix elements of operators transformed with the double similarity transformation and the low-order functional derivatives of the average-value functional. We also derive a fundamental identity concerning the functional derivatives of the average-value functional, and elucidate the consequent recursion relations between the matrix elements of the average-value functional. This section is quite central to the later developments. In Sec. V we derive the equations of motion for the basic amplitudes, first by applying the previously introduced effective-action or dynamical variational principle,[30] and second by a straightforward application of the time-dependent Schrödinger equation with the ECCM parametrization. Both methods are found to lead to the same result. Section VI gives the rules for calculating the average values of products of operators. As a special case of the previous results Sec. VII discusses the commutator of two operators and shows that its average value is given by a generalized Poisson bracket involving only the same first-order functional derivatives as in classical Hamiltonian mechanics. This observation, together with the fact that the ECCM and all amplitudes appearing in it correspond to well-defined and highly linked diagram structures, leads directly to the identification of the method, made in Sec. VIII, as a special kind of bosonization scheme, in which the resulting generalized coherent boson fields have the extreme quality of being classical c-number fields. Lastly, we point out that the ECCM formalism can be given a geometrical interpretation: the basic ECCM amplitudes form a complex symplectic manifold, which is endowed with a Hamiltonian vector field of trajectories describing the temporal flow of the phase-space points. However, only an invariant submanifold of the phase space is in a one-to-one correspondence with the possible physical states of the system.

The ECCM formalism is of very general nature and can be applied to all quantum-mechanical problems for which the Schrödinger dynamics is defined. However, for the purposes of the present paper, we shall henceforth restrict ourselves mostly to bosonic systems as far as concrete examples are concerned, although extensions to systems of fermions or spin-algebraic systems, etc., are in principle quite straightforward. The formalism is presented as for a finite Hilbert space, and we accordingly simply assume convergence in the formal summations over configuration indices.

The present paper I is succeeded by a paper II,[34] which gives a discussion of the excited states and of their connection to the linearized small oscillations around the ground-state configuration. In a later paper we shall discuss an application to the zero-temperature hydrodynamics of a Bose fluid.

II. OPERATOR ALGEBRA IN THE HILBERT SPACE

It is typical of many quantum-mechanical calculations that the construction of states belonging to the full Hilbert space $\mathcal{H}$ is based on some initial or model state $|\Phi\rangle$. This is often chosen to be the ground state that the system would otherwise be in when (some part of) the interactions are turned off. We start here with such a state $|\Phi\rangle$, and assume furthermore that the algebra of all operators in $\mathcal{H}$ is spanned by the two subalgebras of creation and destruction operators with respect to the given model state $|\Phi\rangle$. We assume further that these two subalgebras and the state $|\Phi\rangle$ are cyclic in the sense that all of the ket states in $\mathcal{H}$ can be constructed

from linear combinations of the states reached by operating on $|\Phi\rangle$ with the elements of the creation-operator subalgebra, and that this can also be done for the bra states with respect to the state $\langle\Phi|$.

In what follows we shall assume the state $|\Phi\rangle$ to be a (generalized) vacuum state, examples of which will be given below. This allows one to speak about configuration creation and destruction operators in the standard meaning of the word, and to introduce orthonormal bases, which span the subspaces of creation and destruction operators. Thus, denoting the various configurations by indices $i,j,\ldots$, we shall assume

$$\langle\Phi|C_i C_j^\dagger|\Phi\rangle=\delta(i,j)\ , \tag{2.1}$$

where $\delta(i,j)$ is a Kronecker symbol, and as a consequence of the completeness of the bases the resolution of the identity operator is given by

$$I=|\Phi\rangle\langle\Phi|+\sum_i{}' C_i^\dagger|\Phi\rangle\langle\Phi|C_i$$

$$=\sum_i C_i^\dagger|\Phi\rangle\langle\Phi|C_i\ . \tag{2.2}$$

Here the prime denotes restriction to those $C_i^\dagger$ which create at least one particle ($i\neq 0$), the second summation is a shorthand notation which includes also the projection operator $|\Phi\rangle\langle\Phi|$. The configuration index $i=0$ is used to denote the model state itself, and thus $C_0^\dagger=C_0=I$. We give a few concrete examples.

(i) Bose system with $|\Phi\rangle$ taken to be the vacuum. If the one-particle states are labeled by indices ρ, which form the index set $\mathcal{I}\equiv\{\rho\}$, one can write

$$I=|\Phi\rangle\langle\Phi|+\sum_{n=1}^{\infty}1/n!\sum_{\{\rho_i\}}a_{\rho_1}^\dagger\cdots a_{\rho_n}^\dagger|\Phi\rangle\langle\Phi|a_{\rho_n}\cdots a_{\rho_1}$$

$$=|\Phi\rangle\langle\Phi|+\sum_{n=1}^{\infty}\sum_{\{\rho_i\}}\sum_{\substack{\{m_i\}\\(\rho_i<\rho_{i+1})}}1/(m_1!\cdots m_n!)(a_{\rho_1}^\dagger)^{m_1}\cdots(a_{\rho_n}^\dagger)^{m_n}|\Phi\rangle\langle\Phi|(a_{\rho_n})^{m_n}\cdots(a_{\rho_1})^{m_1} \tag{2.3}$$

in terms of the single-boson creation and destruction operators $a_\rho^\dagger$ and a_ρ, respectively, which obey the usual canonical boson commutation relations, $[a_\rho,a_\sigma]=0$, $[a_\rho,a_\sigma^\dagger]=\delta_{\rho\sigma}$. Hence a typical normalized configuration operator is

$$C_i^\dagger=\prod_\rho\frac{1}{(m_\rho^i!)^{1/2}}(a_\rho^\dagger)^{m_\rho^i}\ , \tag{2.4a}$$

and the configuration index i is a shorthand notation for the set $i=\{m_\rho^i\,|\,\rho\in\mathcal{I}\}=\{m_{\rho_1}^i,m_{\rho_2}^i,\ldots\}$. The common superscript i in the exponents m_ρ in Eq. (2.4a) is intended as a reminder of the configuration index set i to which the exponents belong. Alternatively, in real space we may write

$$C_i^\dagger=\frac{1}{\sqrt{m!}}\prod_{i=1}^{m}a^\dagger(\mathbf{x}_i) \tag{2.4b}$$

and the configuration index is $i=(\mathbf{x}_1,\mathbf{x}_2,\ldots,\mathbf{x}_m)$.

(ii) Number-conserving Bose system with a Bose condensate as the model state,

$$|\Phi\rangle=\frac{1}{\sqrt{N!}}(a_0^\dagger)^N|0\rangle\ . \tag{2.5}$$

Following the notation of example (i), but excluding the condensate index 0 from the set $\{\rho\}$, the normalized number-conserving configuration operators are

$$C_i^\dagger=\left[\frac{(N-n)!}{N!}\right]^{1/2}\prod_\rho\left[\frac{1}{(m_\rho^i!)^{1/2}}(a_\rho^\dagger)^{m_\rho^i}\right]a_0^n\ , \tag{2.6}$$

where $n=\sum_\rho m_\rho^i$, and again $i=\{m_\rho^i\}=\{m_1^i,m_2^i,\ldots\}$.

(iii) Fermi system with $|\Phi\rangle$ a Slater determinant. Let $\{\mu\}$ denote the occupied one-particle states and $\{\rho\}$ the empty ones. We have

$$I=\sum_{m=0}^{N}\frac{1}{m!}\sum_{n=0}^{\infty}\frac{1}{n!}\sum_{\{\mu\}}\sum_{\{\rho\}}a_{\rho_1}^\dagger\cdots a_{\rho_n}^\dagger a_{\mu_1}\cdots a_{\mu_m}|\Phi\rangle\langle\Phi|a_{\mu_m}^\dagger\cdots a_{\mu_1}^\dagger a_{\rho_n}\cdots a_{\rho_1}\ , \tag{2.7}$$

and a normalized configuration operator is

$$C_i^\dagger=\left[\prod_\rho(a_\rho^\dagger)^{n_\rho^i}\right]\left[\prod_\mu(a_\mu)^{m_\mu^i}\right] \tag{2.8}$$

with the correspondence $i=\{n_\rho^i,m_\mu^i\}$ and in terms now of the single-fermion creation and destruction operators, which obey the canonical anticommutation relations. Due to the exclusion principle, of course, the exponents n_ρ^i,m_μ^i can take only the values 0 and 1.

(iv) Spin in an irreducible multiplet. We can take

$$|\Phi\rangle=|J,M=-J\rangle\ , \tag{2.9}$$

and for the normalized configuration operators

$$C_m^\dagger=\left[\frac{(2J-m)!}{(2J)!m!}\right]^{1/2}J_+^m\ ; \tag{2.10}$$

hence

$$C_m^\dagger|J,-J\rangle=|J,-J+m\rangle\ . \tag{2.11}$$

In the case of several similar spins tensorial products of the above operators are used. An important special case is the system of spin $\frac{1}{2}$ particles; the many-body model of Lipkin, Meshkov, and Glick[35] belongs to this class.

Most of the formalism to be presented is completely system independent. The few system-dependent features originate from only one source, which is the explicit form of the modified Wick theorem (Appendix A). Although we shall mostly work specifically with case (i) above, i.e., with a Bose system where $|\Phi\rangle$ is the vacuum, very few changes to the equations appear in other applications, and these cases will be specially mentioned. The abbreviated notation introduced above for the configuration operators is very useful for the formal developments, which otherwise would be very complex looking and case dependent.

Using the above notation an arbitrary ket state $|\Psi\rangle$ in $\mathcal{H}$ can be written as

$$|\Psi\rangle=\sum_i \psi_i C_i^\dagger|\Phi\rangle, \quad \psi_i=\langle\Phi|C_i|\Psi\rangle\ ; \tag{2.12}$$

the bra states can be written similarly.

For later purposes we will find it useful to develop a notation for compounding configuration indices. We shall denote these by the ordinary symbols of addition and subtraction, e.g., $(i+j)$ and $(i-j)$ or $\{[(i+j)-k]+l\}$, etc. From our prior discussion it is clear that these expressions cannot possibly be interpreted in the usual arithmetic sense. Bearing in mind that the configuration indices actually stand for sets of labels for one-particle states, the compounding operations must be understood rather in a set-theoretical sense. Specifically, we define

$$C_{i+j}^\dagger=C_j^\dagger C_i^\dagger, \quad C_{i+j}=C_i C_j\ , \tag{2.13}$$

$$C_{i-j}^\dagger|\Phi\rangle=C_j C_i^\dagger|\Phi\rangle, \quad \langle\Phi|C_{i-j}=\langle\Phi|C_i C_j^\dagger\ . \tag{2.14}$$

Since the operator $C_{i-j}^\dagger$ is thus defined to be the creation part of the full contraction of the product $C_j C_i^\dagger$, it is clear that it is nonzero only if the index set j is a proper subset of the index set i.

In a similar way we define compound-expansion coefficients,

$$\psi_{i+j}=\langle\Phi|C_{i+j}|\Psi\rangle=\sum_k \psi_k\langle\Phi|C_i C_j C_k^\dagger|\Phi\rangle\ , \tag{2.15}$$

$$\psi_{i-j}=\langle\Phi|C_{i-j}|\Psi\rangle=\sum_k \psi_k\langle\Phi|C_i C_j^\dagger C_k^\dagger|\Phi\rangle\ , \tag{2.16}$$

and compound Kronecker symbols, e.g.,

$$\delta(i,j+k)=\langle\Phi|C_i C_k^\dagger C_j^\dagger|\Phi\rangle=\delta(i-k,j)\ . \tag{2.17}$$

The reader should be warned that these operations of addition and subtraction on the configuration indices are generally neither associative nor commutative, e.g., $\psi_{i+(j-k)}\neq\psi_{(i+j)-k}$, although $\psi_{i-(j+k)}=\psi_{(i-j)-k}$. The numerical value of a compound Kronecker symbol is not always 0 or 1. For example, if in Eq. (2.17) the index i contains a multiple occupancy of some one-boson state, and the labels referring to this state are distributed to both j and k and not just one of them, the resulting coefficient is larger than 1. Otherwise the use of the Kronecker symbol is quite straightforward, and we have, e.g.,

$$\sum_i \delta(j,i+k)\psi_i=\sum_i \delta(j-k,i)\psi_i=\psi_{j-k}\ . \tag{2.18}$$

The need for introducing compound configuration indices is intrinsically connected to the nonlinear nature of the exp$S$ method, which splits the full N-body configuration space of the N-body problem into simpler, lower-dimensional, nonlinearly coupled manifolds. Otherwise the operations with the configuration operators and indices would reduce in a trivial way to ordinary linear matrix algebra.

When operators are arranged in normal order, use can be made of the following equation, which can be interpreted as a modification of the Wick theorem:

$$C_j C_i^\dagger=\sum_k Z_k(i,j)C_{i-k}^\dagger C_{j-k}\ . \tag{2.19}$$

Here $Z_k(i,j)$ is a numerical coefficient, which depends on the system in question. For the vacuum Bose system, case (i) above, this factor is

$$Z_k(i,j)=1, \quad \text{case (i)} \tag{2.20}$$

as proven in Appendix A. For the Bose condensate system (ii) the factors $Z_k(i,j)$ differ from 1 by terms which are $O(1/N)$ in magnitude. These other systems are not considered more closely in the present article, but we briefly mention that, e.g., in the case of a Fermi system the configuration indices can be defined such that the coefficients $Z_k(i,j)$ are identically equal to $+1$ or -1. The latter value is obtained in the case when both of the configurations, i and j, are either fermionic or bosonic. Even if both of the indices i and j were bosonic, the application of the Wick theorem would lead to the appearance of fermionic configuration indices. For Fermi systems it is, therefore, natural to allow for odd fermionic configurations right from the beginning in the formalism. The odd configurations should be associated with odd Grassmann ECCM amplitudes. The general average-value functional for a Fermi system is therefore a functional of classical even and odd Grassmann amplitudes.

III. BASIC ECCM AMPLITUDES AND THE AVERAGE-VALUE FUNCTIONAL

The basic formalism of the exp$S$ or coupled-cluster method (CCM) was introduced by Coester and Kümmel in their fundamental papers.[2-3,36] In CCM the ground state is parametrized as

$$|\Psi_0\rangle=e^S|\Phi\rangle\ , \tag{3.1}$$

where S is composed of creation operators (with respect to $|\Phi\rangle$) only. The energy eigenvalue equation

$$H|\Psi_0\rangle=E_0|\Psi_0\rangle \tag{3.2}$$

can thus be written in the form

$$e^{-S}He^S|\Phi\rangle=E_0|\Phi\rangle\ , \tag{3.3}$$

where a similarity transformation of the energy operator is introduced.[2] For a true many-body system there are two major advantages, which make the formulation (3.3) of the ground-state problem attractive in comparison to the conventional equation (3.2): the correct amplitudes S represent sums of linked-cluster diagrams[1-3] and are therefore very convenient in parametrizing $|\Psi_0\rangle$, and the resulting energy E_0 (together with all the individual terms contributing to it) accordingly satisfies the size consistency or size extensivity requirement.[6,18,19]

The exp$S$ similarity transformation has turned out to be invaluable in developing simple and finite algorithms for the evaluation of the ground-state energy. To obtain a satisfactory and energy-compatible algorithm for the calculation of the average values of arbitrary operators diagram analysis suggested the introduction of another set of linked-cluster amplitudes, S'', which generate a second similarity transformation.[30] The resulting extended exp$S$ formulation is thus based on a double similarity transformation rather than a single one. The amplitude S'' is composed only of destruction operators and is again a linked-cluster quantity possessing a well-defined diagrammatic description.[30] The transform of the Hamiltonian is defined as

$$\hat{H}=e^{S''}e^{-S}He^{S}e^{-S''} , \tag{3.4}$$

and the ground-state eigenvalue problem can be written for both the ket and bra eigenstates in a unified way,

$$\hat{H}\,|\Phi\rangle=E_0\,|\Phi\rangle , \tag{3.5}$$

$$\langle\Phi|\,\hat{H}=E_0\langle\Phi|\ . \tag{3.6}$$

The ground states are accordingly introduced in the forms

$$|\Psi_0\rangle=e^{S}|\Phi\rangle=e^{S}e^{-S''}|\Phi\rangle , \tag{3.7}$$

$$\langle\Psi_0'|=\langle\Phi|e^{S''}e^{-S} , \tag{3.8}$$

which satisfy the normalization conditions

$$\langle\Phi|\Psi_0\rangle=1 , \tag{3.9}$$

$$\langle\Psi_0'|\Psi_0\rangle=1 . \tag{3.10}$$

Using the parametrization in terms of the configuration operators of the previous chapter, we write

$$S=\sum_i{}' S_i C_i^{\dagger} , \tag{3.11}$$

$$S''=\sum_i{}' S_i'' C_i . \tag{3.12}$$

It has been pointed out earlier[30] that the set $\{S,S''\}$ is not the most convenient choice for the basic free variables in the extended CCM. Instead, we make a change of free variables to a new set $\{\Sigma,S''\}\equiv\{\Sigma,\tilde{\Sigma}\}$, which we define as follows:

$$\Sigma=\sum_i{}' \sigma_i C_i^{\dagger} , \tag{3.13}$$

$$\tilde{\Sigma}=\sum_i{}' \tilde{\sigma}_i C_i , \tag{3.14}$$

$$\sigma_i=\langle\Phi|C_i e^{S''}S|\Phi\rangle , \tag{3.15}$$

$$\tilde{\sigma}_i=S_i'' . \tag{3.16}$$

The inverse transformation to (3.15) is

$$S_i=\langle\Phi|C_i e^{-\tilde{\Sigma}}\Sigma|\Phi\rangle . \tag{3.17}$$

On defining the functionals

$$\omega_i=\omega_i[\tilde{\sigma}]\equiv\langle\Phi|e^{S''}C_i^{\dagger}|\Phi\rangle , \tag{3.18}$$

$$\bar{\omega}_i=\bar{\omega}_i[\tilde{\sigma}]\equiv\langle\Phi|e^{-S''}C_i^{\dagger}|\Phi\rangle , \tag{3.19}$$

we find

$$\sigma_i=\sum_j{}' S_j\omega_{j-i} , \tag{3.20}$$

$$S_i=\sum_j{}' \sigma_j\bar{\omega}_{j-i} . \tag{3.21}$$

As explained in Sec. II the subtraction of indices is defined to mean

$$\omega_{j-i}\equiv\langle\Phi|e^{S''}C_iC_j^{\dagger}|\Phi\rangle=\frac{\delta}{\delta\tilde{\sigma}_i}\omega_j$$

$$=\langle\Phi|e^{S''}C_{j-i}^{\dagger}|\Phi\rangle . \tag{3.22}$$

We can redefine the indices and write, instead of (3.20),

$$\sigma_i=\sum_k\sum_j{}'\delta(k,j-i)S_j\omega_k$$

$$=\sum_k S_{k+i}\omega_k , \tag{3.23}$$

where use has been made of the rules given in Sec. II.

In expressions (3.20) and (3.21) the indices i and j in ω_{j-i} can be identically equal in which case $\omega_0=\bar{\omega}_0=1$. The transformation matrices have the following orthogonality property:

$$\sum_k\bar{\omega}_{i-k}\omega_{k-j}=\sum_k\omega_{i-k}\bar{\omega}_{k-j}=\delta(i,j) . \tag{3.24}$$

The exp$S$ formalism, in particular in the present extended formulation, is not manifestly Hermitian, since the similarity transformations, which generate the ket and bra ground states, are not unitary. As the discussion of excited states in paper II will emphasize, the formalism actually turns out to be a biorthogonal formulation of the many-body problem. We can identify the quantity $\langle\Phi|\,\hat{A}\,|\Phi\rangle$ as the general average-value functional for an arbitrary operator A, since

$$\langle\Phi|\,\hat{A}\,|\Phi\rangle=\langle\Phi|e^{S''}e^{-S}Ae^{S}|\Phi\rangle$$

$$=\langle\Psi_0'|\,A\,|\Psi_0\rangle , \tag{3.25}$$

and the ground states $\langle\Psi_0'|$ and $|\Psi_0\rangle$ are manifestly normalized according to (3.10). From now on, we shall use the simple notation

$$\langle A\rangle\equiv\langle\Phi|\,\hat{A}\,|\Phi\rangle \tag{3.26}$$

and consider $\langle A\rangle$ to be a functional of either the set $\{S,S''\}$ or the set $\{\Sigma,\tilde{\Sigma}\}$.

We may rewrite Eq. (3.25) in terms of the well-known

nested commutator expansion, as

$$\langle A \rangle = \sum_n \frac{1}{n!} \langle \Phi | e^{S^{\dagger}} A\{S;n\} | \Phi \rangle , \tag{3.27}$$

where

$$A\{S;0\} = A, \quad A\{S;n\} = [A\{S;n-1\},S], \quad n \geq 1 . \tag{3.28}$$

Following the notation of Kümmel *et al.*,[4] we write Eq. (3.27) in the equivalent form,

$$\langle A \rangle = \sum_n \frac{1}{n!} \langle \Phi | e^{S^{\dagger}} \{AS^n\}_L | \Phi \rangle , \tag{3.29}$$

where the notation $\{AS^n\}_L$ means that from each S there must be at least one link (contraction) to the operator A. The sum over n extends to a finite limit depending on the operator A. It has been shown earlier[30] that the structure of the average-value functional in terms of the new variables $\Sigma, \bar{\Sigma}$ can be expressed in the form

$$\begin{aligned} \langle A \rangle &= \langle \Phi | e^{\bar{\Sigma}} e^{-\Sigma} A e^{\Sigma} | \Phi \rangle_{\mathrm{DL}} \\ &= \sum_n \frac{1}{n!} \langle \Phi | e^{\bar{\Sigma}} \{A\Sigma^n\}_L | \Phi \rangle_{\mathrm{DL}} , \end{aligned} \tag{3.30}$$

where the subscript DL (double or definite linking) imposes a further restriction on the linking structure; namely, after expanding in powers of $\bar{\Sigma}$ only such terms are retained where each $\bar{\Sigma}$ is linked at least to two different amplitudes Σ, unless $\bar{\Sigma}$ is linked directly to the operator A. We can write

$$\begin{aligned} \langle A \rangle = \sum_{n,m} \frac{1}{n!m!} \sum_{\{i\}}{}' \sum_{\{j\}}{}' & \langle i_1 \cdots i_m | A | j_1 \cdots j_n \rangle \\ & \times \bar{\sigma}_{i_1} \cdots \bar{\sigma}_{i_m} \sigma_{j_n} \cdots \sigma_{j_1} , \end{aligned} \tag{3.31}$$

where the matrix elements $\langle \cdots | A | \cdots \rangle$ obey the above definite linking restrictions. The explicit expressions for the matrix elements are given in Appendix B. They satisfy a simple but important recursion formula, also given in Appendix B, which is based on the identity to be derived in Sec. IV.

Figure 1(a) gives an abbreviated pictorial representation of the average-value functional $\langle A \rangle$. At this stage of the analysis, the diagram simply indicates the linked or connected structure of $\langle A \rangle$. It is only after the equations of motion have been considered with proper boundary conditions that these diagrams can be interpreted as the usual equilibrium diagrams of perturbation theory. It is perhaps worth pointing out that the present approach is quite the converse of the usual perturbation-theory approach, where the equilibrium is first assumed and the corresponding diagrams introduced immediately. This latter approach is then difficult to extend to the case of symmetry breaking or topological deformation of the assumed equilibrium; whereas our own approach retains a greater degree of flexibility.

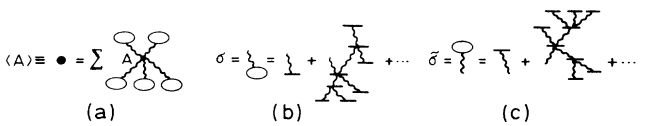

FIG. 1. (a) Pictorial representation of Eq. (3.31) for the average value $\langle A \rangle$ of an operator A as a functional of the amplitudes σ and $\bar{\sigma}$. A wavy line denotes a many-body configuration. (b)–(c) The GTO tree structure of the amplitudes σ and $\bar{\sigma}$ at the stationary point. The small bars denote the vertices of the Hamiltonian operator and the wavy lines are now free many-body propagators.

An analysis of the linking structure of the average values $\langle C_i^{\dagger} \rangle$ of the creation operators shows that the new amplitudes $\bar{\sigma}_i$ are precisely the linked parts of such averages. Of particular importance is the energy functional $\langle H \rangle$, which determines the dynamics of the amplitudes $\{\sigma, \bar{\sigma}\}$ and their ground-state equilibrium values. At the stationary point the values of $\sigma_j, \bar{\sigma}_j$ represent the contributions of definite classes of linked Goldstone diagrams. These can be classified in a convenient way in terms of extended GTO trees,[30] the structures of which are described in Figs. 1(b) and 1(c). The precise meaning and examples of the pictorial representation of the vertices of the Hamiltonian have been discussed elsewhere.[30] Here we will be satisfied with a brief recapitulation of the main results of the diagram analysis.

An extended ground-state GTO diagram [like the ones in Figs. 1(b) and 1(c)] is composed of two kinds of elements: the Hamiltonian vertices represented by small horizontal bars, and the links (wavy lines) connecting the vertices. The links form tree structures, and therefore between any pair of vertices there exists a unique route of links. The links represent static on-energy-shell free many-body propagators and to each link there thus is associated an on-energy-shell energy denominator factor. By definition, the relative lengths of the links are irrelevant; only the time directions of the links matter.

Each wavy line or link with a given configuration index i is thus a set of one-body propagator lines. The structure of an allowed Hamiltonian vertex can be specified by requiring that (i) from each link entering the vertex from below at least one link is directly connected to the operator H (or V), (ii) from each link emerging up from the vertex either at least one line is connected directly to H or, if no lines are so connected, there must be one-body lines to at least two different wavy links below the vertex. These limitations are just the DL conditions mentioned above (in Ref. 30 the notation *ll* limited linking was used for DL). For a more detailed description of the vertices, see Sec. V. 3 in Ref. 30.

The ground-state energy shift ΔE is given by the sum of all closed extended GTO tree diagrams. Each such diagram represents the sum of a definite class of Goldstone diagrams, in which the relative time orders of the Hamiltonian vertices of the Goldstone diagrams are allowed to vary in a particular way. The extended GTO diagrams in fact introduce a summation scheme which is

in a definite sense intermediate between the Goldstone diagrams and Feynman diagrams. Cutting a link in a closed extended GTO diagram gives two open extended GTO diagrams [cf. Figs. 1(b) and 1(c)], which form possible contributions to the amplitudes $\bar{\sigma}$ and σ. Taking into account the overall connectedness of the closed extended GTO diagram together with the DL restrictions at the vertices it is clear that all the diagrams for the ground-state amplitudes $\bar{\sigma}$ and σ are connected.

IV. FUNCTIONAL DERIVATIVES AND MATRIX ELEMENTS OF TRANSFORMED OPERATORS

There is a close connection between the functional derivatives of the average value of an operator and the matrix elements of the transformed operator. To elucidate this connection let us define the notation for the various functional derivatives as follows:

$$\frac{\delta f}{\delta S_i}=\frac{\delta f[S,S'']}{\delta S_i}\bigg|_{S''};\quad \frac{\delta f}{\delta S_i''}=\frac{\delta f[S,S'']}{\delta S_i''}\bigg|_{S}, \tag{4.1}$$

$$\frac{\delta f}{\delta \sigma_i}=\frac{\delta f[\Sigma,\tilde{\Sigma}]}{\delta \sigma_i}\bigg|_{\tilde{\Sigma}};\quad \frac{\delta f}{\delta \bar{\sigma}_i}=\frac{\delta f[\Sigma,\tilde{\Sigma}]}{\delta \bar{\sigma}_i}\bigg|_{\Sigma}. \tag{4.2}$$

Using equations (3.16) and (3.18)–(3.21) we find

$$\frac{\delta}{\delta S_i}=\sum_j{}'\,\omega_{i-j}\frac{\delta}{\delta \sigma_j}, \tag{4.3}$$

$$\frac{\delta}{\delta S_i''}=\frac{\delta}{\delta \bar{\sigma}_i}+\sum_j{}'\,\sigma_{i+j}\frac{\delta}{\delta \sigma_j}. \tag{4.4}$$

As an application of the use of these expressions we calculate the matrix element ($i\neq 0$)

$$\begin{aligned}\langle\Phi\mid C_i\hat{A}\mid\Phi\rangle&=\langle\Phi\mid C_i e^{S''}e^{-S}Ae^{S}\mid\Phi\rangle\\&=\frac{\delta}{\delta S_i''}\langle\Phi\mid\hat{A}\mid\Phi\rangle\\&=\frac{\delta\langle A\rangle}{\delta\bar{\sigma}_i}+\sum_j{}'\,\sigma_{i+j}\frac{\delta\langle A\rangle}{\delta\sigma_j}.\end{aligned} \tag{4.5}$$

The next example is the element ($i\neq 0$)

$$\begin{aligned}\langle\Phi\mid\hat{A}C_i^{\dagger}\mid\Phi\rangle&=\langle\Phi\mid e^{S''}e^{-S}Ae^{S}(I)e^{-S''}C_i^{\dagger}\mid\Phi\rangle\\&=\langle A\rangle\bar{\omega}_i+\sum_j{}'\,\bar{\omega}_{i-j}\langle\Phi\mid e^{S''}e^{-S}Ae^{S}C_j^{\dagger}\mid\Phi\rangle\\&=\langle A\rangle\bar{\omega}_i+\sum_j{}'\,\bar{\omega}_{i-j}\{\langle\Phi\mid e^{S''}e^{-S}[A,C_j^{\dagger}]e^{S}\mid\Phi\rangle+\langle\Phi\mid e^{S''}C_j^{\dagger}e^{-S''}(I)e^{S''}e^{-S}Ae^{S}\mid\Phi\rangle\}\\&=\langle A\rangle\bar{\omega}_i+\sum_j{}'\,\bar{\omega}_{i-j}\left[\frac{\delta\langle A\rangle}{\delta S_j}+\langle A\rangle\omega_j+\sum_k{}'\,\langle\Phi\mid e^{S''}C_j^{\dagger}e^{-S''}C_k^{\dagger}\mid\Phi\rangle\langle\Phi\mid C_k\hat{A}\mid\Phi\rangle\right].\end{aligned} \tag{4.6}$$

Above we have inserted the resolution of identity (2.2) into the places which are denoted by (I). The final step is to use the results (4.3), (3.24), and (4.5) to obtain

$$\begin{aligned}\langle\Phi\mid\hat{A}C_i^{\dagger}\mid\Phi\rangle&=\frac{\delta\langle A\rangle}{\delta\sigma_i}+\sum_{j,k}{}'\,\frac{\delta\langle A\rangle}{\delta\sigma_j}\sigma_{j+k}L_{ki}\\&\quad+\sum_j{}'\,\frac{\delta\langle A\rangle}{\delta\bar{\sigma}_j}L_{ji},\end{aligned} \tag{4.7}$$

where we define (for $i\neq 0\neq j$) the new amplitude

$$\begin{aligned}L_{ij}=L_{ji}&=\sum_{k,l}\omega_{k+l}\bar{\omega}_{i-k}\bar{\omega}_{j-l}\\&=\sum_{k,l}\langle\Phi\mid e^{S''}C_k^{\dagger}C_l^{\dagger}\mid\Phi\rangle\langle\Phi\mid C_k e^{-S''}C_i^{\dagger}\mid\Phi\rangle\\&\quad\times\langle\Phi\mid C_l e^{-S''}C_j^{\dagger}\mid\Phi\rangle.\end{aligned} \tag{4.8}$$

It will be instructive to analyze the diagrammatic meaning of the matrix L_{ij}. By summing over the configurations l and using the closure relation (2.2) we find

$$\begin{aligned}L_{ij}&=\sum_k\langle\Phi\mid e^{S''}C_k^{\dagger}e^{-S''}C_j^{\dagger}\mid\Phi\rangle\langle\Phi\mid C_k e^{-S''}C_i^{\dagger}\mid\Phi\rangle\\&=\sum_k\sum_n 1/n!\langle\Phi\mid\{(S'')^n C_k^{\dagger}\}_L C_j^{\dagger}\mid\Phi\rangle\\&\quad\times\langle\Phi\mid C_k e^{-S''}C_i^{\dagger}\mid\Phi\rangle,\end{aligned} \tag{4.9}$$

where the obvious generalization of the notation of Ref. 4, Eq. (3.29), this time signifies that from each S'' there must be a link to the operator $C_k^{\dagger}$. We find the following:

(i) Every line of the group $C_j^{\dagger}$ is connected to some S'' amplitude, arising from the factor $e^{S''}$, and

(ii) from every such S'' amplitude arising from the factor $e^{S''}$ there is a link to the group $C_k^{\dagger}$, which link propagates directly to the group $C_i^{\dagger}$.

As a consequence we find that every line rising up from the group $C_j^{\dagger}$ is linked to the group $C_i^{\dagger}$ through some such S'' amplitude. If the sum over k is performed first

in the expression (4.8), we get the reciprocal statement: every line of the group $C_i^\dagger$ is linked to the group $C_j^\dagger$ through an S'' amplitude arising from the factor $e^{S''}$.

The result is that all possible amplitudes $(-S'')$ arising from the exponential $\exp(-S'')$ cancel against other similar more weakly linked diagrams, and the final outcome can be cast in the form

$$L_{ij} = \langle \Phi \mid e^{\bar{\Sigma}} C_i^\dagger C_j^\dagger \mid \Phi \rangle_{\mathrm{DL}} = \sum_n 1/n! \langle \Phi \mid \{ (\bar{\Sigma})^n C_i^\dagger C_j^\dagger \}_{\mathrm{DL}} \mid \Phi \rangle \ . \tag{4.10}$$

The DL symbol again signifies strong linking, namely, that every $\bar{\Sigma}$ appearing must be linked both to $C_i^\dagger$ and to $C_j^\dagger$.

As a warning to the reader we perform also an erroneous analysis of the expression (4.8). Let us choose new indices $m = i-k$, $n = j-l$, hence

$$L_{ij} = \sum_m \sum_n \omega_{(i-m)+(j-n)} \bar{\omega}_m \bar{\omega}_n \ .$$

If we now ignored what was said after Eq. (2.17) in Sec. II and assumed $\omega_{(i-m)+(j-n)} = \omega_{i-m+j-n} = \omega_{i+j-m-n}$, we would get

$$L_{ij}^{\mathrm{false}} = \sum_m \sum_n \langle \Phi \mid e^{S''} C_n C_m C_i^\dagger C_j^\dagger \mid \Phi \rangle \times \langle \Phi \mid e^{-S''} C_m^\dagger \mid \Phi \rangle \langle \Phi \mid e^{-S''} C_n^\dagger \mid \Phi \rangle$$

$$= \langle \Phi \mid e^{-S''} C_i^\dagger C_j^\dagger \mid \Phi \rangle = \bar{\omega}_{i+j}$$

on using again the closure relation.

Next we calculate the matrix element (for $i \neq 0 \neq j$)

$$\begin{aligned}
\langle \Phi \mid C_i \hat{A} C_j^\dagger \mid \Phi \rangle &= \langle \Phi \mid C_i e^{S''} e^{-S} A e^{S} (I) e^{-S''} C_j^\dagger \mid \Phi \rangle \\
&= \langle \Phi \mid C_i \hat{A} \mid \Phi \rangle \bar{\omega}_j + \sum_k{}' \langle \Phi \mid C_i e^{S''} e^{-S} A e^{S} C_k^\dagger \mid \Phi \rangle \bar{\omega}_{j-k} \\
&= \langle \Phi \mid C_i \hat{A} \mid \Phi \rangle \bar{\omega}_j + \sum_k{}' \bar{\omega}_{j-k} \{ \langle \Phi \mid C_i e^{S''} e^{-S} [A, C_k^\dagger] e^{S} \mid \Phi \rangle \\
&\quad + \sum_l \sum_m \langle \Phi \mid C_i e^{S''} C_k^\dagger C_l^\dagger \mid \Phi \rangle \langle \Phi \mid C_l e^{-S''} C_m^\dagger \mid \Phi \rangle \langle \Phi \mid C_m e^{S''} e^{-S} A e^{S} \mid \Phi \rangle \} \\
&= \langle \Phi \mid C_i \hat{A} \mid \Phi \rangle \bar{\omega}_j + \sum_k{}' \bar{\omega}_{j-k} \left[\frac{\delta^2 \langle A \rangle}{\delta S_k \delta S_i''} + \sum_l \sum_m \omega_{(k+l)-i} \bar{\omega}_{m-l} \left[\delta(m,0) \langle A \rangle + \frac{\delta \langle A \rangle}{\delta S_m''} \right] \right] .
\end{aligned} \tag{4.11}$$

By applying the rules (4.3) and (4.4) and the orthogonality relations (3.24) we readily get (for $i \neq 0 \neq j$)

$$\langle \Phi \mid C_i \hat{A} C_j^\dagger \mid \Phi \rangle = \langle A \rangle \delta(i,j) + \frac{\delta \langle A \rangle}{\delta \sigma_{j-i}} + \sum_k{}' \frac{\delta \langle A \rangle}{\delta \sigma_k} \sum_l{}' \sigma_{k+l} L_{lj}^i + \sum_k{}' \frac{\delta \langle A \rangle}{\delta \bar{\sigma}_k} L_{kj}^i + \sum_k{}' \frac{\delta^2 \langle A \rangle}{\delta \sigma_j \delta \sigma_k} \sigma_{k+i} + \frac{\delta^2 \langle A \rangle}{\delta \bar{\sigma}_i \delta \sigma_j} , \tag{4.12}$$

where the coefficient is defined as

$$\begin{aligned}
L_{jk}^i = L_{kj}^i &= \sum_l \sum_m \omega_{(l+m)-i} \bar{\omega}_{j-l} \bar{\omega}_{k-m} \\
&= \sum_l \sum_m \langle \Phi \mid e^{S''} C_i C_l^\dagger C_m^\dagger \mid \Phi \rangle \langle \Phi \mid e^{-S''} C_l C_j^\dagger \mid \Phi \rangle \\
&\quad \times \langle \Phi \mid e^{-S''} C_m C_k^\dagger \mid \Phi \rangle \ .
\end{aligned} \tag{4.13}$$

Another way to derive the matrix element (4.12) is to observe that

$$\langle \Phi \mid C_i \hat{A} C_j^\dagger \mid \Phi \rangle = \langle \Phi \mid \hat{A} C_i C_j^\dagger \mid \Phi \rangle + \frac{\delta}{\delta S_i''} \langle \Phi \mid \hat{A} C_j^\dagger \mid \Phi \rangle \tag{4.14}$$

and to use the result (4.7) and Eq. (4.4). In simplifying the emerging expressions use must be made of the fact that

$$\frac{\delta^2 \langle A \rangle}{\delta S_i'' \delta S_j''} = \langle \Phi \mid C_i C_j \hat{A} \mid \Phi \rangle = \frac{\delta \langle A \rangle}{\delta S_{i+j}''} , \tag{4.15}$$

which leads to the following important identity:

$$\frac{\delta \langle A \rangle}{\delta \bar{\sigma}_{i+j}} = \frac{\delta^2 \langle A \rangle}{\delta \bar{\sigma}_i \delta \bar{\sigma}_j} + \sum_k{}' \left[\sigma_{i+k} \frac{\delta^2 \langle A \rangle}{\delta \sigma_k \delta \bar{\sigma}_j} + \frac{\delta^2 \langle A \rangle}{\delta \bar{\sigma}_i \delta \sigma_k} \sigma_{k+j} \right] + \sum_k{}' \sum_l{}' \sigma_{i+k} \frac{\delta^2 \langle A \rangle}{\delta \sigma_k \delta \sigma_l} \sigma_{l+j} \ . \tag{4.16}$$

This basic identity will be frequently needed in simplifying functional-derivative expressions, e.g., in connection with the study of excited states (paper II). It leads to a recursion formula between the matrix elements of the average-value functional, which is spelled out in Appendix B.

The final step in simplifying the right-hand side of (4.14) makes use of the identification

$$L^i_{jk}=\frac{\delta L_{jk}}{\delta\tilde{\sigma}_i}+L_{j,k-i}+L_{j-i,k}\ , \tag{4.17}$$

which can be directly verified by comparing the definitions (4.8) and (4.13).

By using the modified Wick theorem (2.19) it is possible to write down the coefficient L^i_{jk} entirely in terms of the L_{lm} matrices,

$$L^i_{jk}=\sum_{l,m}L_{j-l,k-m}\delta(l+m,i)\ . \tag{4.18}$$

The proof of this result is given in Appendix A. The above result is valid for the vacuum Bose system only and will be modified by extra factors in the case of other systems. The result is easy to understand, because the matrices L_{ij} are exponential forms of $\tilde{\sigma}$ in spite of the double-linking requirements; therefore the functional derivatives reduce to similar exponential forms.

We give in Fig. 2 a pictorial presentation of the amplitudes L_{jk} and L^i_{jk}. The diagrammatic content of L^i_{jk} is most easy to see from Eq. (4.17). The first term is the result when an $\tilde{\sigma}_i$ amplitude is erased from L_{jk}; the configuration group i therefore has links both to j and to k, and the remaining $\tilde{\sigma}$ amplitudes are also strongly linked. The second and the third terms correspond to cases when the whole i group is taken from either j or k.

The main results of the present section are the expressions (4.5), (4.7), and (4.12) for the matrix elements of $\hat{A}$, as well as the identity (4.16). We also shall illustrate these results by diagrammatical representation. Let the functional derivatives of the average value $\langle A\rangle$ with respect to σ_i and $\tilde{\sigma}_i$ be denoted as in Fig. 3 by loose ends signifying the erased amplitudes. Then we get Figs. 4–6 for the matrix elements and Fig. 7 for the identity (4.16).

The ground state is defined by the condition that the first-order functional derivatives of $\langle H\rangle$ with respect to the amplitudes $\sigma,\tilde{\sigma}$ must be zero.[30] Applied to the identity (4.16) this requirement yields a condition on the second-order functional derivatives of the Hamiltonian, which is similar in form to the random-phase approximation (RPA) of the standard CCM.[11,24] Just as in the standard RPA case, the present equation can be iterated to give a resolution of σ_{i+j} with a compound index in terms of an expansion in the second-order derivatives of $\langle H\rangle$. This is shown in Fig. 8.

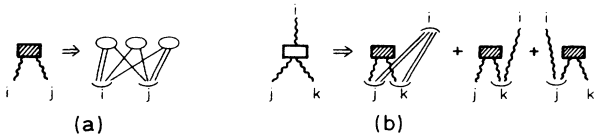

FIG. 2. Diagrammatic description of (a) L_{jk} from Eq. (4.10) and (b) L^i_{jk} from Eq. (4.17).

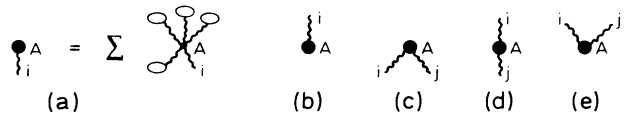

FIG. 3. Pictorial representation of the functional derivatives (a) $\delta\langle A\rangle/\delta\sigma_i$, (b) $\delta\langle A\rangle/\delta\tilde{\sigma}_i$, (c) $\delta^2\langle A\rangle/\delta\sigma_i\delta\sigma_j$, (d) $\delta^2\langle A\rangle/\delta\tilde{\sigma}_i\delta\sigma_j$, and (e) $\delta^2\langle A\rangle/\delta\tilde{\sigma}_i\delta\tilde{\sigma}_j$. A tail on the dot, which represents $\langle A\rangle$ as in Fig. 1, denotes a functional derivative.

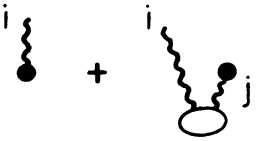

FIG. 4. Representation of matrix element $\langle\Phi|C_i\hat{A}|\Phi\rangle$ of Eq. (4.5) in terms of functional derivatives.

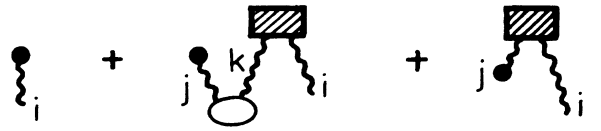

FIG. 5. Representation of matrix element $\langle\Phi|\hat{A}C_i^\dagger|\Phi\rangle$ of Eq. (4.7) in terms of functional derivatives.

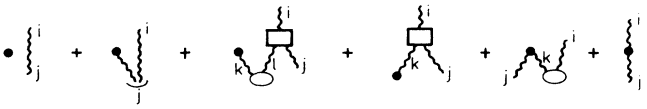

FIG. 6. Representation of matrix element $\langle\Phi|C_i\hat{A}C_j^\dagger|\Phi\rangle$ in terms of functional derivatives. The diagrams correspond term by term with those in Eq. (4.12).

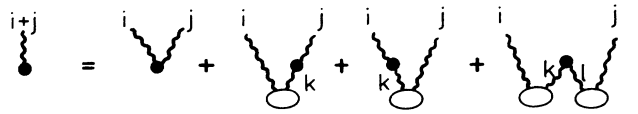

FIG. 7. Representation of the identity in Eq. (4.16) concerning the functional derivatives.

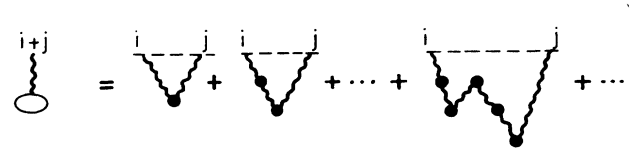

FIG. 8. The diagrammatic structure of σ_{i+j} in the ground state. The dots with tails are the second-order functional derivatives of $\langle H\rangle$, as in Fig. 3, and their time levels must precede the uppermost open end level, where the horizontal dashed line signifies the presence of the energy-denominator factor. Compare this with the structure of σ given in Fig. 1(b).

V. EQUATIONS OF MOTION

A. Dynamical variational principle

The equations of motion for the ECCM amplitudes are obtained from a variational principle by requiring the actionlike functional

$$\mathcal{A}=\int dt\,\langle\Phi\mid e^{S''(t)}e^{-S(t)}[i\partial/\partial t-H(t)]e^{S(t)}\mid\Phi\rangle \quad (5.1)$$

to be stationary against small variations of the amplitudes.[30] In the time-independent case the stationary conditions yield the eigenvalue equations (3.5)–(3.8), assuming the states $\mid\Phi\rangle$ and $\langle\Phi\mid$ to be cyclic with respect to the creation- and annihilation-operator subalgebras. In the general case the stationary conditions lead to the dynamical evolution equations for the amplitudes $\{S,S''\}$ or $\{\Sigma,\tilde{\Sigma}\}$.

In terms of the pair $\{\Sigma,\tilde{\Sigma}\}$ the action functional becomes

$$\begin{aligned}\mathcal{A}&=\int dt[i\langle\Phi\mid\tilde{\Sigma}\dot{\Sigma}\mid\Phi\rangle-\langle\Phi\mid\hat{H}\mid\Phi\rangle]\\&=\int dt\left[i\sum_j{}'\tilde{\sigma}_j\dot{\sigma}_j-\langle H\rangle\right]\\&=\int dt[-i\langle\Phi\mid\dot{\tilde{\Sigma}}\Sigma\mid\Phi\rangle-\langle\Phi\mid\hat{H}\mid\phi\rangle]\\&=\int dt\left[-i\sum_j{}'\dot{\tilde{\sigma}}_j\sigma_j-\langle H\rangle\right].\end{aligned} \quad (5.2)$$

The stationary conditions then yield the pair of equations of motion,

$$i\dot{\sigma}_j=\left.\frac{\delta\langle\Phi\mid\hat{H}\mid\Phi\rangle}{\delta\tilde{\sigma}_j}\right|_{\Sigma}, \quad (5.3)$$

$$i\dot{\tilde{\sigma}}_j=-\left.\frac{\delta\langle\Phi\mid\hat{H}\mid\Phi\rangle}{\delta\sigma_j}\right|_{\tilde{\Sigma}}. \quad (5.4)$$

B. Time-dependent Schrödinger equation

We can arrive at the same equations of motion in a straightforward manner by using an ECCM parametrization for the time-development operators in the Schrödinger picture. These are assumed to be given in the form

$$U(t)=e^{\phi(t)}e^{S(t)}e^{-S''(t)},\quad \mid\Psi(t)\rangle=U(t)\mid\Phi\rangle, \quad (5.5)$$

$$\tilde{U}(t)=e^{-\tilde{\phi}(t)}e^{S''(t)}e^{-S(t)},\quad \langle\Psi'(t)\mid=\langle\Phi\mid\tilde{U}(t), \quad (5.6)$$

where ϕ and $\tilde{\phi}$ are c numbers. From the Schrödinger equations for the ket and bra states,

$$i\frac{\partial}{\partial t}\mid\Psi(t)\rangle=H\mid\Psi(t)\rangle, \quad (5.7)$$

$$-i\frac{\partial}{\partial t}\langle\Psi'(t)\mid=\langle\Psi'(t)\mid H, \quad (5.8)$$

the following intermediate results are derived:

$$i\dot{\phi}\mid\Phi\rangle+ie^{S''}\dot{S}\mid\Phi\rangle=\hat{H}\mid\Phi\rangle, \quad (5.9)$$

$$i\dot{\tilde{\phi}}\langle\Phi\mid-i\langle\Phi\mid\dot{S}''+i\langle\Phi\mid e^{S''}\dot{S}e^{-S''}=\langle\Phi\mid\hat{H}. \quad (5.10)$$

We wish to substitute for the amplitudes S the new Σ, and by using Eqs. (3.19) and (3.21) we obtain

$$\dot{S}_k=\sum_l{}'\dot{\sigma}_l\bar{\omega}_{l-k}-\sum_l{}'\dot{\tilde{\sigma}}_l\sum_m{}'\sigma_m\bar{\omega}_{(m-k)-l}. \quad (5.11)$$

On substituting this expression into Eq. (5.9) and taking the scalar product with the state $\langle\Phi\mid C_a$ one finally gets the result

$$i\dot{\sigma}_a-\frac{\delta\langle H\rangle}{\delta\tilde{\sigma}_a}-\sum_b{}'\sigma_{a+b}\left[i\dot{\tilde{\sigma}}_b+\frac{\delta\langle H\rangle}{\delta\sigma_b}\right]=0, \quad (5.12)$$

where use has been made of the orthogonality of the matrices ω and $\bar{\omega}$, Eq. (3.24), as well as Eq. (4.5).

In the same way we take the scalar product of Eq. (5.10) with the state $C_a^{\dagger}\mid\Phi\rangle$, and use Eqs. (5.11) and (4.7)–(4.8) to obtain the result

$$-i\dot{\tilde{\sigma}}_a-\frac{\delta\langle H\rangle}{\delta\sigma_a}+\sum_b{}'L_{ab}\left[i\dot{\sigma}_b-\frac{\delta\langle H\rangle}{\delta\tilde{\sigma}_b}-\sum_c{}'\sigma_{b+c}\left[i\dot{\tilde{\sigma}}_c+\frac{\delta\langle H\rangle}{\delta\sigma_c}\right]\right]=0. \quad (5.13)$$

The expression multiplying L_{ab} above is identically zero due to Eq. (5.12). What remains in Eq. (5.13) is the same equation of motion as in Eq. (5.4). Inserting this into Eq. (5.12), where it multiplies σ_{a+b}, the other equation of motion (5.3) follows.

It is also of interest to calculate the equations of motion for ϕ and $\tilde{\phi}$ which give the size factors e^{ϕ} and $e^{-\tilde{\phi}}$. They can be found by taking scalar products of Eq. (5.9) and (5.10) with $\langle\Phi\mid$ and $\mid\Phi\rangle$, respectively. By now the technique should be quite standard, and we just state the results

$$i\dot{\phi}=\langle H\rangle+\sum_a{}'\left[\frac{\delta\langle H\rangle}{\delta\tilde{\sigma}_a}\bar{\omega}_a+\frac{\delta\langle H\rangle}{\delta\sigma_a}(S_a-\sigma_a)\right], \quad (5.14)$$

$$\dot{\tilde{\phi}}=\dot{\phi}. \quad (5.15)$$

Therefore the scalar product

$$\langle\Psi'(t)\mid\Psi(t)\rangle=\exp[\phi(t)-\tilde{\phi}(t)] \quad (5.16)$$

remains constant in time, and proper normalization is obtained by setting $\tilde{\phi}=\phi$.

VI. AVERAGE VALUES OF OPERATOR PRODUCTS

An arbitrary product of operators transforms under the double similarity transformation into the corresponding product of transformed operators. Thus, if $R=ABC\cdots$, then

$$\hat{R} \equiv e^{S''} e^{-S} ABC \cdots e^{S} e^{-S''} = \hat{A}\hat{B}\hat{C} \cdots \ . \tag{6.1}$$

The average value of the product is therefore

$$\langle ABC \cdots \rangle = \langle \Phi \mid \hat{A}\hat{B}\hat{C} \cdots \mid \Phi \rangle \ . \tag{6.2}$$

On inserting the resolution of the identity operator (2.2) between each entry, and using the results of Sec. IV, it is possible to express the average value of a product in terms of functional derivatives of the average values of individual factors, with coefficients that are functionals of Σ and $\bar{\Sigma}$. The functional derivatives appearing in such expressions are at most of second order.

The most important case is the product of two operators,

$$\langle AB \rangle = \langle A \rangle \langle B \rangle + \sum_i{}' \langle \Phi \mid \hat{A} C_i^{\dagger} \mid \Phi \rangle \langle \Phi \mid C_i \hat{B} \mid \Phi \rangle \ . \tag{6.3}$$

Using the results (4.5) and (4.7) we find

$$\langle AB \rangle = \langle A \rangle \langle B \rangle + \sum_i{}' \sum_j{}' \left[\frac{\delta \langle A \rangle}{\delta \sigma_i} \frac{\delta \langle B \rangle}{\delta \sigma_j} X_{ij}^{11} + \frac{\delta \langle A \rangle}{\delta \sigma_i} \frac{\delta \langle B \rangle}{\delta \bar{\sigma}_j} X_{ij}^{12} + \frac{\delta \langle A \rangle}{\delta \bar{\sigma}_i} \frac{\delta \langle B \rangle}{\delta \sigma_j} X_{ij}^{21} + \frac{\delta \langle A \rangle}{\delta \bar{\sigma}_i} \frac{\delta \langle B \rangle}{\delta \bar{\sigma}_j} X_{ij}^{22} \right] , \tag{6.4}$$

where the coefficients are given by

$$X_{ij}^{11} = X_{ji}^{11} = \sigma_{i+j} + \sum_k{}' \sum_l{}' \sigma_{i+k} L_{kl} \sigma_{l+j} \ , \tag{6.5}$$

$$X_{ij}^{12} = \delta(i,j) + \sum_k{}' \sigma_{i+k} L_{kj} \ , \tag{6.6}$$

$$X_{ij}^{21} = \sum_k{}' L_{ik} \sigma_{k+j} \ , \tag{6.7}$$

$$X_{ij}^{22} = X_{ji}^{22} = L_{ij} \ . \tag{6.8}$$

The terms for the average value of the product are presented diagrammatically in Fig. 9. For our present purposes we need not study the more complicated cases of products of more than two operators, or the average values of functions of operators.

VII. COMMUTATORS AND GENERALIZED POISSON BRACKETS

As a particularly important application of the results of Sec. VI we now consider the expectation value of the commutator of two operators. In view of the high degree of symmetry exhibited in Eqs. (6.5)–(6.8) by the X coefficients, there is a considerable consequent simplification in this regard. We find

$$\langle \Psi_0' \mid (AB - BA) \mid \Psi_0 \rangle \equiv \langle [A,B] \rangle = i \{ \overline{A}, \overline{B} \} \ , \tag{7.1}$$

where the generalized Poisson bracket $\{ \overline{A}, \overline{B} \}$ is defined by

$$i \{ \overline{A}, \overline{B} \} \equiv \sum_j{}' \left[\frac{\delta \overline{A}}{\delta \sigma_j} \frac{\delta \overline{B}}{\delta \bar{\sigma}_j} - \frac{\delta \overline{B}}{\delta \sigma_j} \frac{\delta \overline{A}}{\delta \bar{\sigma}_j} \right] , \tag{7.2}$$

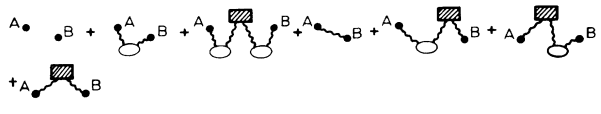

FIG. 9. Graphical representation of the average value $\langle AB \rangle$ from Eq. (6.4) in terms of functional derivatives.

and where we have now used the bar to indicate the average-value functional, $\langle A \rangle \equiv \overline{A} \equiv \overline{A}[\sigma, \bar{\sigma}]$, in order to simplify the notation.

This result can be made even more suggestive by choosing as new basic variables the generalized fields ϕ_i and their canonically conjugate generalized momentum densities π_i, defined as

$$\phi_i \equiv (\tfrac{1}{2})^{1/2} (\sigma_i + \bar{\sigma}_i) \ , \tag{7.3}$$

$$\pi_i \equiv i (\tfrac{1}{2})^{1/2} (\bar{\sigma}_i - \sigma_i) \ . \tag{7.4}$$

In this way we can redefine the average values $\langle A \rangle$ as functionals of ϕ and π, in terms of which Eq. (7.2) becomes

$$\{ \overline{A}, \overline{B} \} = \sum_j{}' \left[\frac{\delta \overline{A}}{\delta \phi_j} \frac{\delta \overline{B}}{\delta \pi_j} - \frac{\delta \overline{B}}{\delta \phi_j} \frac{\delta \overline{A}}{\delta \pi_j} \right] . \tag{7.5}$$

In terms of the new amplitudes the equations of motion (5.3) and (5.4) are thereby recast into the form

$$\frac{d\phi_i}{dt} = \{ \phi_i, \overline{H} \} = \frac{\delta \overline{H}}{\delta \pi_i} \ , \tag{7.6}$$

$$\frac{d\pi_i}{dt} = \{ \pi_i, \overline{H} \} = -\frac{\delta \overline{H}}{\delta \phi_i} \ . \tag{7.7}$$

Finally, for an arbitrary, intrinsically time-dependent operator $A(t)$, it is straightforward to show, using Eqs. (7.5)–(7.7), that the equation of motion for its average-value functional $\overline{A}[\phi, \pi; t]$ is

$$\frac{d}{dt} \overline{A} = \frac{\overline{\partial A}}{\partial t} + \{ \overline{A}, \overline{H} \} \ , \tag{7.8}$$

which is the well-known classical equation of motion in the canonical formalism. Using the definition in Eq. (7.1) of the Poisson bracket, Eq. (7.8) is found to give the proper quantum-mechanical equation of motion for the average value,

$$\frac{d \langle A \rangle}{dt} = \left\langle \frac{\partial A}{\partial t} \right\rangle + \frac{1}{i} \langle [A,H] \rangle \ . \tag{7.9}$$

The consistency of the classical and quantum formula-

tions can be understood as a manifestation of the correspondence principle in a suitable generalized form.

We are thus led to the important result that the whole of our quantum many-body problem has formally been exactly mapped onto the classical Hamiltonian mechanics for the (c number) quasilocal fields ϕ_i and π_i which are themselves functions in the many-body configuration space labeled by the indices i. In this way we can take over (or suitably extend) the whole of the classical formalism to describe (exactly, in principle, if no truncations are made) the quantum many-body system. In particular we can make easy contact with such things as conservation laws and the associated sum rules. These aspects will be discussed in a future paper.

VIII. EXACT BOSONIZATION AND THE ECCM PHASE SPACE

Among the most important degrees of freedom describing a complex many-body system are the slow, long-wavelength modes which traditionally are parametrized in terms of collective coordinates. We have seen how our basic ECCM amplitudes achieve a natural interpretation as classical quasilocal fields obeying a classical Hamiltonian mechanics. In this light, it is very natural to expect the ECCM fields to have a close connection with generalized collective coordinates. The extraction of the proper collective variables from the basic microscopic theory has been of great interest especially in nuclear physics. One way towards this goal has proceeded through various bosonization methods.

There is a long tradition in the bosonization of spin-algebraic or fermionic systems. As examples of the genre we mention the methods of Holstein and Primakoff,[37] Dyson,[38] Schwinger[39] and others[12,40–42] and refer the reader to the review by Garbaczewski.[43] The basic philosophy in these methods has been to map the original Hilbert space of the system $\mathcal{H}$ into a boson Hilbert space $\mathcal{H}^B$. The boson images of suitably chosen pairs of fermion operators (or spin operators) are constructed in such a fashion that the Lie-algebra structure of the original operators in $\mathcal{H}$ and of the image operators in $\mathcal{H}^B$ is identical. In all the approaches referred to above the boson Hilbert space $\mathcal{H}^B$ turns out to be too large in the sense that physically realizable states in the original space map into a subspace of $\mathcal{H}^B$. Thus the dynamics in $\mathcal{H}^B$ reflects faithfully the original dynamics in $\mathcal{H}$ only if one restricts oneself to this physical subspace of $\mathcal{H}^B$. A further point to notice is that depending on the details of the chosen mapping of $\mathcal{H}$ into $\mathcal{H}^B$, the boson Hamiltonian H^B can be either Hermitian or non-Hermitian.[41] In some cases one can also offer a diagrammatic meaning to the bosonization. An example of this kind is the treatment of the electron gas as a collection of interacting Sawada bosons, i.e., electron-hole pair excitations.[42] This Dyson-type bosonization scheme leads to a non-Hermitian Hamiltonian H^B, and one can regard the Sawada bosons appearing in the bosonic perturbation diagrams as corresponding to approximate excited linked configurations of the original fermionic system.

As emphasized earlier, one of the main goals in applying a bosonization method is to find such a description of the original fermionic system that the chosen boson operators in $\mathcal{H}^B$, at least for the low-lying collective excitations, can be treated almost as noninteracting ideal bosons. In a general case, however, there exist nontrivial, residual, quantal interactions between the bosons, and the boson-expansion method is a mathematically complicated theory of mutually interacting bosons in a projected subspace of $\mathcal{H}^B$.

The ECCM theory discussed in the present paper is, when truncated at its lowest level of approximation, the so-called SUB1 approximation where in the expansions (3.13) and (3.14) for the amplitudes Σ and $\tilde{\Sigma}$ the sums over configurations are restricted to one-body configurations i only, precisely equal to the mean field theory or semiclassical approximation.[30] For the bosonic systems, which have mainly been emphasized here, this is precisely the ordinary coherent-state approximation, while for fermionic systems it would correspond to the Hartree-Fock approximation. In the case of bosons this approximation can be expressed in terms of the (classical) coherent states of Glauber.[44,45] Using the complete set of our original single-boson creation and destruction operators $a^\dagger(\mathbf{x})$ and $a(\mathbf{x})$ [see discussion after Eq. (2.3)], we define the Glauber coherent state as

$$|g\rangle = e^G|\Phi\rangle , \tag{8.1}$$

where the generator G is

$$G = \int d^3x[\phi(\mathbf{x})a^\dagger(\mathbf{x}) - \phi^*(\mathbf{x})a(\mathbf{x})] = -G^\dagger \tag{8.2}$$

and $\phi(\mathbf{x})$ and its complex conjugate $\phi^*(\mathbf{x})$ are scalar (i.e., c-number) fields, and with $|\Phi\rangle$ the vacuum, $a(\mathbf{x})|\Phi\rangle = 0$, as before. It is straightforward to show that

$$a(\mathbf{x})e^G|\Phi\rangle = \phi(\mathbf{x})e^G|\Phi\rangle , \tag{8.3}$$

$$\langle\Phi|e^{-G}a^\dagger(\mathbf{x}) = \phi^*(\mathbf{x})\langle\Phi|e^{-G} . \tag{8.4}$$

The expectation value of a normal-ordered arbitrary operator $A =: A[a,a^\dagger]:$ in these coherent states is just given by replacing the field operators $a(\mathbf{x})$ and $a^\dagger(\mathbf{x})$ in the functional by their c-number coherent-state expectation values $\phi(\mathbf{x})$ and $\phi^*(\mathbf{x})$, respectively,

$$\langle A\rangle_G \equiv \langle\Phi|e^{-G}:A[a,a^\dagger]:e^G|\Phi\rangle = \overline{A}[\phi,\phi^*] . \tag{8.5}$$

In particular we can calculate the dynamics of the system at this SUB1 level from the coherent-state action functional

$$\mathcal{A}^G = \int dt\{i\int d^3x\phi^*(\mathbf{x})\dot{\phi}(\mathbf{x}) - \overline{H}[\phi,\phi^*]\} , \tag{8.6}$$

where $\overline{H}[\phi,\phi^*]$ is the Hamiltonian functional of the system in the SUB1 approximation.

Although the preceding treatment of the boson system, using Glauber coherent states, is clearly an approximation, we could go a step further and apply the fact that the coherent states $|g\rangle$ form an over-complete set of states and express the exact ground state of the system as a superposition of these states $|g\rangle$ and effectively transform the exact Schrödinger equation (3.2) into an

integral equation. The solution of this Hill-Wheeler equation would then give us the exact ground-state wave function and energy. Here we do not pursue this idea any further, but instead show how the exact, nontruncated ECCM approach can be formulated as a generalized mean field theory.

We now formalize the ideas discussed above by introducing ideal bosonic annihilation and creation operators $\alpha_i,\tilde{\alpha}_i$ associated with each configuration i, such that they satisfy the canonical commutation relations

$$[\alpha_i,\alpha_j]=[\tilde{\alpha}_i,\tilde{\alpha}_j]=0, \quad [\alpha_i,\tilde{\alpha}_j]=\delta(i,j) . \tag{8.7}$$

We postulate the existence of the vacuum states $|\Phi_B\rangle$ and $\langle\Phi'_B|$ by requiring

$$\alpha_i|\Phi_B\rangle\equiv 0, \quad \langle\Phi'_B|\tilde{\alpha}_i\equiv 0 , \tag{8.8}$$

and assume these states to be cyclic with respect to the algebra of the operators $\{\alpha,\tilde{\alpha}\}$. Thus an entire boson Hilbert space $\mathcal{H}^B$ can be constructed by successive operations on the vacuum states with the canonical operators.

For every operator A in $\mathcal{H}$ we then associate its boson image A^B in $\mathcal{H}^B$, defined as

$$A^B\equiv\sum_{m,n}\frac{1}{m!n!}\sum_{\{i\}}'\sum_{\{j\}}'\langle i_1\cdots i_m|A|j_1\cdots j_n\rangle \times\tilde{\alpha}_{i_1}\cdots\tilde{\alpha}_{i_m}\alpha_{j_n}\cdots\alpha_{j_1} , \tag{8.9}$$

where the matrix element is exactly as specified previously in Eq. (3.31) or in Appendix B.

The coherent (or bicoherent) states in $\mathcal{H}^B$ can be given in the form $e^{\Gamma}|\Phi_B\rangle,\langle\Phi'_B|e^{-\Gamma}$, where the generator is

$$\Gamma=\sum_i'(\sigma_i\tilde{\alpha}_i-\tilde{\sigma}_i\alpha_i) . \tag{8.10}$$

We readily find that the average values of the basic canonical operators in a bicoherent state are

$$\langle\alpha_i\rangle\equiv\langle\Phi'_B|e^{-\Gamma}\alpha_i e^{\Gamma}|\Phi_B\rangle=\sigma_i , \tag{8.11a}$$

$$\langle\tilde{\alpha}_i\rangle\equiv\langle\Phi'_B|e^{-\Gamma}\tilde{\alpha}_i e^{\Gamma}|\Phi_B\rangle=\tilde{\sigma}_i , \tag{8.11b}$$

and for an arbitrary boson image of the form (8.9) one obtains

$$\langle A^B\rangle\equiv\langle\Phi'_B|e^{-\Gamma}A^B[\tilde{\alpha},\alpha]e^{\Gamma}|\Phi_B\rangle=A^B[\tilde{\sigma},\sigma] . \tag{8.12}$$

But this expression is identical to the previously considered ECCM average-value functional $\langle A\rangle$ of Eq. (3.31), when the coupled-cluster operators S and S'' are parametrized by the amplitudes $\sigma,\tilde{\sigma}$.

It is then natural to introduce the generalized coherent-state action functional $\mathcal{A}^B$, defined in the boson space $\mathcal{H}^B$ to be

$$\mathcal{A}^B=\int dt\,\langle\Phi'_B|e^{-\Gamma(t)}\left[i\frac{\partial}{\partial t}-H^B\right]e^{\Gamma(t)}|\Phi_B\rangle . \tag{8.13}$$

By making use of the result

$$e^{-\Gamma}\frac{\partial}{\partial t}e^{\Gamma}=\frac{\partial}{\partial t}I+\left[\frac{\partial}{\partial t},\Gamma\right]+\frac{1}{2!}\left[\left[\frac{\partial}{\partial t},\Gamma\right],\Gamma\right] =\frac{\partial}{\partial t}I+\sum_i'[\dot{\sigma}_i\tilde{\alpha}_i-\dot{\tilde{\sigma}}_i\alpha_i+\tfrac{1}{2}(\dot{\sigma}_i\tilde{\sigma}_i-\sigma_i\dot{\tilde{\sigma}}_i)] , \tag{8.14}$$

which follows from Eqs. (8.7) and (8.10), we finally find the result that $\mathcal{A}^B$ has a form identical to our earlier result in Eq. (5.2),

$$\mathcal{A}^B=\int dt\left[i\sum_j'\tilde{\sigma}_j\dot{\sigma}_j-H^B[\tilde{\sigma},\sigma]\right] . \tag{8.15}$$

Hence, a variational principle applied to the action $\mathcal{A}^B$ exactly reproduces our earlier (exact) equations of motion (5.3) and (5.4) for the ECCM amplitudes $\sigma,\tilde{\sigma}$.

We therefore come to the conclusion that the totality of the original ECCM states $e^S|\Phi\rangle,\langle\Phi|e^{S''}e^{-S}$ can be mapped onto the subset of coherent states $e^{\Gamma}|\Phi_B\rangle,\langle\Phi'_B|e^{-\Gamma}$ in an ideal boson Hilbert space. The mapping is one to one and allows straightforward introduction of the rules for the average-value functional as well as for the dynamical behavior. Thus, in a very definite sense, the present *generalized coherent bosonization* as described above, is an *exact bosonization* of the original system, in contrast, for example, to the usual (Glauber) coherent states, which only give an approximation to the state of a system.

It is of interest to discuss the general features of the present exact bosonization scheme in particular with reference to other conventional bosonization methods. In the present case we have a well-defined diagrammatical interpretation for the Bose fields in terms of maximally linked diagram structures, and the consequent quasilocality property. In this respect the method resembles the Sawada bosonization of a Fermi system, or the Dyson bosonization of a (pseudo)spin-algebraic system. We could go so far as to claim that the present bosonization is a generalization of the Dyson scheme. In both cases the mapping to the Bose space is non-Hermitian and the diagram structures at the vertices have common features.

The essential difference to all the other methods is that in our case the concept of bosonization is taken to the logical extreme, namely, the boson fields obtained are classical c numbers and accordingly no longer possess quantum-mechanical interactions. The only interactions which appear are classical nonlinear couplings between the fields. But this property can, indeed, be understood to be the ultimate goal of the bosonization methods. For increasingly complicated configuration indices i the field amplitudes $\sigma_i,\tilde{\sigma}_i$ may loosely be viewed as a sequence of collective coordinates of increasing complexity, which eventually yield an exact description for all collective degrees of freedom, at least when properly diagonalized. This point is elaborated further in paper II.

As a further difference to standard methods the present scheme can be applied to all quantum-mechanical problems in a unified fashion, and not only

to fermion or spin-algebraic systems. Thus, for example, boson systems can also be bosonized in our scheme. Since the resulting exact bosonized description is a classical field theory, it cannot be bosonized any further.

Since the physical states in the ideal boson space are coherent states, and a superposition of two or more coherent states is generally not a coherent state, the physical bosonized states do not form a subspace in $\mathcal{H}^B$. Accordingly, the superposition principle does not apply between the physical states $\mathcal{H}^B$. This, of course, is connected to the fact that the bosonized description is no longer a genuine quantum theory, but instead a classical, effective field theory.

Another manifestation of this particular aspect is the fact that the Lie algebra of operators is not exactly preserved in the present bosonization scheme. Thus, in general, we have the inequality

$$([A_1, A_2])^B \neq [A_1^B, A_2^B] , \tag{8.16}$$

where the first commutator between the original operators A_1 and A_2 is calculated in $\mathcal{H}$, and the second commutator of the boson images, of the form given by Eq. (8.9), is calculated in $\mathcal{H}^B$. However, the Lie algebra is exactly preserved, if the full boson commutators are restricted to the *tree level* to be specified below. We therefore have

$$([A_1, A_2])^B = [A_1^B, A_2^B]_{\text{tree}} . \tag{8.17}$$

The tree level of a commutator is defined to be a restriction to such contractions where no closed loops are allowed. The tree commutator is thus obtained in $\mathcal{H}^B$ by allowing only one pair of $\alpha_i, \tilde{\alpha}_j$ to be contracted at a time, and arranging the remaining boson operators in normal order.

As an example, consider the operators $A_1^B = \tilde{\alpha}_1\alpha_2\alpha_3$, $A_2^B = \tilde{\alpha}_4\tilde{\alpha}_5\alpha_6$. The full commutator can be written, after arranging into normal order, as

$$\begin{aligned}[A_1^B, A_2^B] =: \{ & \tilde{\alpha}_1\underbrace{\alpha_2\alpha_3\tilde{\alpha}_4}\tilde{\alpha}_5\alpha_6 + \tilde{\alpha}_1\underbrace{\alpha_2\alpha_3\tilde{\alpha}_4}\tilde{\alpha}_5\alpha_6 \\ & + \tilde{\alpha}_1\alpha_2\underbrace{\alpha_3\tilde{\alpha}_4}\tilde{\alpha}_5\alpha_6 + \tilde{\alpha}_1\alpha_2\alpha_3\underbrace{\tilde{\alpha}_4\tilde{\alpha}_5}\alpha_6 \\ & + \tilde{\alpha}_1\underbrace{\alpha_2\alpha_3\tilde{\alpha}_4}\tilde{\alpha}_5\alpha_6 + \tilde{\alpha}_1\underbrace{\alpha_2\alpha_3\tilde{\alpha}_4}\tilde{\alpha}_5\alpha_6 \\ & - \tilde{\alpha}_4\tilde{\alpha}_5\underbrace{\alpha_6\tilde{\alpha}_1}\alpha_2\alpha_3 \} : \end{aligned} \tag{8.18}$$

where the contraction $\underbrace{\alpha_i\tilde{\alpha}_j}$ above is naturally defined to be $\delta(i,j)$. At the tree level we omit the first two terms, which contain double contractions between the vertices of A_1^B and A_2^B leading to closed loops. The remaining terms are

$$\begin{aligned}[A_1^B, A_2^B]_{\text{tree}} & \\ =: \{ & \tilde{\alpha}_1\alpha_2\underbrace{\alpha_3\tilde{\alpha}_4}\tilde{\alpha}_5\alpha_6 + \tilde{\alpha}_1\alpha_2\underbrace{\alpha_3\tilde{\alpha}_4}\tilde{\alpha}_5\alpha_6 + \tilde{\alpha}_1\underbrace{\alpha_2\alpha_3\tilde{\alpha}_4}\tilde{\alpha}_5\alpha_6 \\ & + \tilde{\alpha}_1\underbrace{\alpha_2\alpha_3\tilde{\alpha}_4}\tilde{\alpha}_5\alpha_6 - \tilde{\alpha}_4\tilde{\alpha}_5\underbrace{\alpha_6\tilde{\alpha}_1}\alpha_2\alpha_3 \} : . \end{aligned} \tag{8.19}$$

These results are illustrated in Figs. 10(a) and 10(b), respectively.

Evidently, these peculiar rules for the commutators in the bosonized picture follow from the expressions for the matrix elements $\langle i_1 \cdots i_m \mid A_1 A_2 \mid j_1 \cdots j_n \rangle$ of the product of operators and of their commutators, as explained in Secs. VI and VII, respectively. The subsequent nonappearance of closed-loop diagrams is a further reflection of the fact that we have succeeded in exactly reformulating the original quantum-mechanical many-body system as a classical generalized mean-field theory.

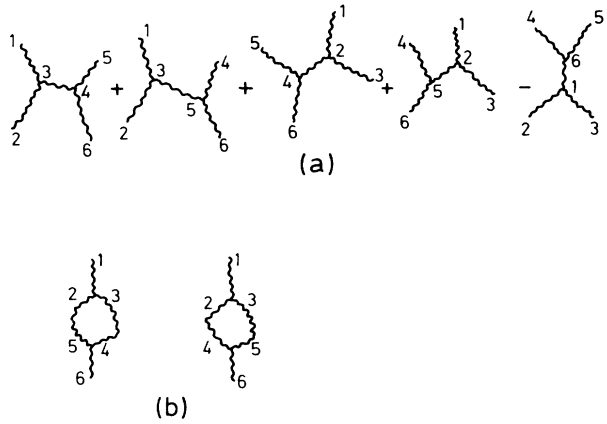

FIG. 10. Pictorial representation of (a) the tree-level commutator of the operators $\tilde{\alpha}_1\alpha_2\alpha_3$ and $\tilde{\alpha}_4\tilde{\alpha}_5\alpha_6$ in Eq. (8.19) and (b) the extra loop terms in their full commutator, given by the first two terms of Eq. (8.18).

As was briefly mentioned in Sec. II, the most consistent way to introduce the ECCM parametrization for the fermion systems allows also fermionic configurations comprising an odd number of particles and the odd Grassmann amplitudes $\sigma, \tilde{\sigma}$ associated with such configurations. In the ground state or any collectively excited state satisfying the superselection rule, which forbids even and odd configurations in the same wave function, such odd Grassmann amplitudes are then zero. As was pointed out earlier[30] and will be described more thoroughly in paper II, the small fluctuations of the even amplitudes are connected with even fermionic collective excitations. Correspondingly, the small fluctuations of the odd amplitudes will be related to the odd fermionic (e.g., single-particle) excitations, for which reason it is vital to allow for infinitesimal breakings of the superselection rule. Generalizing to larger virtual breakings, we actually are led to speak not only of exact coherent bosonization, but also of *exact coherent fermionization.* The general bosonized and fermionized Hamiltonian, or its average value in the generalized coherent state, is a classical effective Hamiltonian composed of even and odd classical Grassmann fields.

One final aspect of the ECCM deserves to be mentioned. As has been thoroughly discussed above, the method transforms an arbitrary quantum theory in a Hilbert space into a classical field theory in a classical ECCM phase space. The coordinates in this phase space are the fields $\sigma_i, \tilde{\sigma}_i$, or the canonical fields ϕ_i and momenta π_i, Eqs. (7.3) and (7.4). The phase space can be more precisely characterized by observing that in the modern terminology of classical mechanics it is a symplectic differentiable manifold.[46] The differentiability is a consequence of the fact that the numerical values of

the fields ϕ_i,π_i are continuous complex numbers, and one is accordingly allowed to take (functional) derivatives with respect to the fields. The property of being symplectic is a consequence of the existence of the Poisson bracket, i.e., a skew-symmetric bilinear form, which can be used to define a Hamiltonian vector field in the tangent space of the manifold.[46] In more ordinary language, the equations of motion define a set of trajectories, which fill the whole dynamically allowed region of the phase space.

The requirement that the physical states in the original Hilbert space should satisfy the Hermiticity condition

$$\langle \Phi \mid e^{S''} e^{-S} \propto (e^{S} \mid \Phi \rangle)^{\dagger} = \langle \Phi \mid e^{S^{\dagger}} \tag{8.20}$$

leads to a constraint among the amplitudes $\sigma_i,\tilde{\sigma}_i$. The observable physical phase space is thereby only a submanifold in the full ECCM symplectic phase space. It is an invariant submanifold in the sense that it is formed of entire trajectories; either none or all of the points of a trajectory belong to the physical submanifold, assuming the Hamiltonian to be Hermitian. Time development thus leaves this submanifold invariant. Even within this submanifold the amplitudes σ_i and $\tilde{\sigma}_i$ are not complex conjugates of each other, because the ECCM similarity transformations are not unitary. Only by performing a suitable complex canonical transformation can one recover a description in terms of real coordinates ϕ_i',π_i' instead of complex ones.

It almost goes without saying that the geometrical or topological properties of the full ECCM phase space are immensely more complicated than in the usual classical mechanics of continuous media. Roughly speaking, the neighborhood of an arbitrary point in the phase space reveals the same complexity as the full original Hilbert space. Nevertheless, due to the quasilocal nature of the ECCM parametrization, one might realistically hope that only a small part of the full phase space turns out to be relevant; i.e., that there occurs "compactification" into a simpler, physically relevant submanifold. In a favorable case there may exist a suitable infrared scale compared to which the description looks completely local and not more complicated than the usual classical mechanics of continuous fields. We shall, however, not expand on this subject in the present article.

IX. SUMMARY AND DISCUSSION

We first briefly summarize the main results of the preceding sections and then offer a more detailed discussion on some separate points of interest.

We have shown how the ECCM parametrization of the Hilbert space may in principle be applied to all such systems for which a Schrödinger dynamics is defined. Effectively, this parametrization can be viewed as an exact mapping of the original quantum-mechanical problem onto a well-defined nonlocal classical field theory in the symplectic ECCM phase space; i.e., "quantum theory is made classical." The coordinates of this ECCM phase space are quasilocal complex c-number fields $\sigma_i,\tilde{\sigma}_i$, which, for example in the case of a Bose system in coordinate space, are n-point functions of the position vectors $(\mathbf{x}_1,\mathbf{x}_2,\ldots,\mathbf{x}_n)$, with $n=1,2,\ldots$. The lowest-order linked-cluster amplitudes $\sigma_1(\mathbf{x})$ and $\tilde{\sigma}_1(\mathbf{x})$ are clearly local by definition, being just average values of the single-particle operators $a(\mathbf{x})$ and $a^{\dagger}(\mathbf{x})$ at position $\mathbf{x}$, whereas quasilocality for the higher-order fields follows from the maximal connectivity built into the ECCM theory. At the stationary point of the system these amplitudes $\sigma_i,\tilde{\sigma}_i$ can be endowed with a diagrammatic interpretation in terms of maximally linked GTO tree diagrams. However, in contrast to the usual diagrammatic approaches based on the assumption of an equilibrium state, we have here developed a more flexible theory that incorporates a more direct means to discuss broken symmetries, topological excitations, and possibly even systems that possess no equilibrium states.

The average values of various physically important operators and products of them are expressible as functionals of the basic amplitudes $\sigma_i,\tilde{\sigma}_i$, and arbitrary matrix elements of such operators can be evaluated as functional derivatives of the corresponding average-value functional in a straightforward manner. The dynamics of the system again is determined by the Hamiltonian functional via the equations of motion for the basic fields $\sigma_i,\tilde{\sigma}_i$. Especially useful in view of the structure of ECCM is the observation that the commutator of two quantum-mechanical operators is mapped into a generalized Poisson bracket of the average-value functionals of the respective operators. It is precisely this feature that endows the ECCM phase space with its symplectic structure.

In Sec. VIII we present the ECCM theory formally as an exact generalized mean-field approach, where the original system is described in terms of generalized coherent bosons α_i and $\tilde{\alpha}_i$, whose expectation values equal the c-number fields $\sigma_i,\tilde{\sigma}_i$. These fields σ_i and $\tilde{\sigma}_i$ can, loosely speaking, be interpreted as collective coordinates of the system, as will become clearer in the forthcoming paper II.

It is of interest to compare our ECCM approach with the well-known density-functional theory of Hohenberg, Kohn, and Sham.[47,48] This latter approach attempts to construct the total energy as a functional of a local parameter, namely, the particle number density $\rho(\mathbf{x})$. In its simplest forms (e.g., the Thomas-Fermi approximation), density-functional theory gives the total energy as a completely local functional of $\rho(\mathbf{x})$. Much of the later effort in this field has gone into the construction of suitable nonlocal extensions to these simple local approximations. In this light the ECCM may be viewed as a rather different framework for incorporating these nonlocal corrections in a completely well-defined manner.

Although the ECCM is in principle exact, approximations or truncations will naturally need to be made in practice, and here again the "maximal connectivity" feature of the basic building blocks leads to many advantages. For purposes of illustration it is interesting to compare the ECCM with both the normal CCM (Refs. 2–6) and the CI method.[17] Each of the three methods can be formulated in terms of suitable sets of classical configuration-space fields σ_i and $\tilde{\sigma}_i$, which obey

Hamilton's equations of motion as we have discussed for the ECCM here. Only in the ECCM, however, are both entire sets quasilocal in the sense of obeying the cluster property. In the normal CCM each member of one set of fields (namely, the amplitudes S_i associated with the single similarity transformation operator S, which parametrizes the ket ground state as $|\Psi_0\rangle = e^S|\Phi\rangle$) is connected; but the other set Ω_i (associated with the bra ground-state parametrization as $\langle\Psi_0'| = \langle\Phi|\Omega e^{-S}$) is not connected. (We note that for an evaluation of the ground-state energy only the amplitudes S_i are needed since one may utilize the Schrödinger equation to avoid use of the bra state $\langle\Psi_0'|$; but both sets S_i and Ω_i are needed to evaluate the ground-state expectation value of an arbitrary operator.) Finally, in the CI method neither the creation nor the destruction amplitudes are connected; and we note that it is just this feature which leads to the size-extensivity problem.[6,18,19]

These various connectivity features of the basic amplitudes are intimately associated with the generalized time-ordering (GTO) properties of each method when restricted to time-independent perturbation theory and the associated Goldstone diagrams. Thus, the normal CCM can be shown to generate generalized tree diagram structures with GTO in the "past" (backward-going) direction only, whereas the ECCM also contains GTO into the "future" (forward-going) direction.[30] By contrast, the CI method has no GTO properties. Now, when any of the methods is truncated, as each must be in practice, these GTO properties assume considerable importance. A typical truncation scheme might be the so-called SUBn approximation wherein the configuration-space indices $\{i\}$ are restricted to involve at most n particles (or particle-hole pairs). In a CI calculation the truncation index n would typically need to be quite large for good accuracy (i.e., the limbs of the associated CI tree diagrams would need to be quite "thick"), unless the interaction is so weak that low-order perturbation theory is sufficient. By contrast, both the normal CCM and ECCM usually achieve comparable accuracy with much lower values of n, and the limbs of their respective tree diagrams need not be so thick (i.e., need not contain so many particles). In the ECCM, the SUB1 approximation is just classical mean field theory (namely, the coherent-state approximation for bosons or Hartree-Fock theory for fermions), whereas the SUB2 approximation for bosons is equivalent to the Gaussian approximation of quantum field theory.[30,49]

We also note that the maximum incorporation of the cluster property for all its basic amplitudes, which is the hallmark of the ECCM, should particularly facilitate its applicability to a description of such topological excitations as the vortex lines in liquid ^{4}He. Such excitations are created by appropriate topological boundary conditions for the basic amplitudes σ_i and $\tilde{\sigma}_i$, which prevent their decay by any quasilocal processes. In such cases, the boundary conditions can only be properly imposed in a theory where the cluster property is exactly obeyed by all of the relevant amplitudes. Typically the boundary condition is imposed at some sufficiently large distance (e.g., from the vortex core in the case of a vortex line), and then since the amplitudes $\sigma_n(\mathbf{x}_1,\ldots,\mathbf{x}_n)$ and $\tilde{\sigma}_n(\mathbf{x}_1,\ldots,\mathbf{x}_n)$ contain no contributions from large interparticle separations for $n>1$, the physics must ultimately be dominated by the amplitudes σ_1 and $\tilde{\sigma}_1$.

The discussion in this paper has focused mainly on the ground state of the quantal system under consideration. It is quite possible to extend the ground-state ECCM to include excited states in analogy to the way Emrich[21] has developed the normal CCM. This extension is the main topic in paper II, where we show explicitly the intimate connection of the excited states with small oscillations around the ground-state configurations obtained by the formalism discussed here. Paper II thus contains an exact theory of linear response within the ECCM.

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APPENDIX A: THE MODIFIED WICK THEOREM

Wick's theorem gives the rules for arranging products of operators into normal order. If the operators A_i are linear and homogeneous in the basic canonical single-particle creation and destruction operators, the theorem gives the standard rule

$$A_1A_2A_3A_4\cdots A_n = :A_1A_2A_3A_4\cdots A_n: + :\underbrace{A_1A_2}A_3A_4\cdots A_n: + \cdots + :\underbrace{A_1A_2}A_3\underbrace{A_4\cdots A_p}A_q\cdots A_n: + \cdots + :\underbrace{A_1A_2}\underbrace{A_3A_4\cdots}A_n: , \tag{A1}$$

where the pairwise contractions are defined as $\underbrace{A_1A_2} = \langle\Phi|A_1A_2|\Phi\rangle$, and : : denotes normal ordering.

We shall show that for the case of boson algebra we can recast the theorem in the following simple form for the product of two configuration operators:

$$C_iC_j^\dagger = \sum_k C_{j-k}^\dagger C_{i-k} , \tag{A2}$$

in the notation of Sec. II.

As the first step we prove (A2) for one single quantum state ρ. To avoid confusion we write for the *normalized* operators ($m=1,2,\ldots$)

$$C_{[m]}^\dagger \equiv 1/\sqrt{m!}\,(a_\rho^\dagger)^m . \tag{A3}$$

Thus $C_m = C_{[m]}, C_m^\dagger = C_{[m]}^\dagger$, but for *combined* indices, due to definition (2.14), we have

$$C_m C_n^\dagger \mid 0\rangle = C_{n-m}^\dagger \mid 0\rangle = \left[\frac{n!}{m!}\right]^{1/2} \frac{1}{(n-m)!}(a_\rho^\dagger)^{n-m} \mid 0\rangle = \begin{bmatrix} n \\ m \end{bmatrix}^{1/2} C_{[n-m]}^\dagger \mid 0\rangle \ . \tag{A4}$$

Here $C_{[n-m]}^\dagger$ is the normalized operator corresponding to the index $l = n-m$, where $n-m$ is just an arithmetic expression rather than a set-theoretical notation.

The rule for combined indices is therefore

$$C_{n-m}^\dagger = \begin{bmatrix} n \\ m \end{bmatrix}^{1/2} C_{[n-m]}^\dagger \ . \tag{A5}$$

The right-hand side of Eq. (A2) is thus

$$\sum_k C_{j-k}^\dagger C_{i-k} = \sum_k \left[\begin{bmatrix} j \\ k \end{bmatrix} \begin{bmatrix} i \\ k \end{bmatrix} \right]^{1/2} C_{[j-k]}^\dagger C_{[i-k]} = \sum_k \left[\begin{bmatrix} j \\ k \end{bmatrix} \begin{bmatrix} i \\ k \end{bmatrix} \frac{1}{(i-k)!(j-k)!} \right]^{1/2} \times (a_\rho^\dagger)^{j-k}(a_\rho)^{i-k} \ , \tag{A6}$$

whereas the left-hand side is

$$C_i C_j^\dagger = 1/\sqrt{i!j!}(a_\rho)^i (a_\rho^\dagger)^j \ . \tag{A7}$$

We show expressions (A6) and (A7) to be equal by applying them to an arbitrary state $\mid n\rangle$. Expression (A6) gives

$$\begin{aligned} \sum_k C_{j-k}^\dagger C_{i-k} \mid n\rangle &= \sum_k \left[\begin{bmatrix} i \\ k \end{bmatrix} \begin{bmatrix} j \\ k \end{bmatrix} \frac{1}{(i-k)!(j-k)!} \right]^{1/2} \left[\frac{n!(n-i+j)!}{(n-i+k)!(n-i+k)!} \right]^{1/2} \mid n-i+j\rangle \\ &= \mid n-i+j\rangle \left[\frac{j!n!}{i!(n-i+j)!} \right]^{1/2} \sum_k \begin{bmatrix} i \\ k \end{bmatrix} \begin{bmatrix} n-i+j \\ j-k \end{bmatrix} \\ &= \mid n-i+j\rangle \left[\frac{j!n!}{i!(n-i+j)!} \right]^{1/2} \begin{bmatrix} n+j \\ j \end{bmatrix} , \end{aligned} \tag{A8}$$

where in the last step use was made of Eq. 0.1561 of Ref. 50. Expression (A7) gives

$$C_i C_j^\dagger \mid n\rangle = \frac{1}{\sqrt{i!j!}} \left[\frac{(n+j)!(n+j)!}{n!(n-i+j)!} \right]^{1/2} \mid n+j-i\rangle \ . \tag{A9}$$

Comparison of the coefficients in (A8) and (A9) shows that they are equal, which proves the Wick theorem (A2) for the single quantum state.

The general case of many quantum states is proven in a straightforward manner by observing Eq. (2.4a), which gives

$$C_i C_j^\dagger = \prod_\rho [C_{m_\rho^i}(\rho) C_{m_\rho^j}^\dagger(\rho)] \ , \tag{A10}$$

where

$$C_m(\rho) = \frac{1}{\sqrt{m!}}(a_\rho)^m \ . \tag{A11}$$

Notice that the configuration index i in this case is equivalent to the set $\{m_\rho^i\} = \{m_{\rho_1}^i, m_{\rho_2}^i, \ldots\}$. Each factor now gives, according to (A2),

$$C_{m_\rho^i}(\rho) C_{m_\rho^j}^\dagger(\rho) = \sum_{m_\rho^k} C_{m_\rho^j - m_\rho^k}^\dagger(\rho) C_{m_\rho^i - m_\rho^k}(\rho) \ , \tag{A12}$$

and the whole product may be rewritten as

$$C_i C_j^\dagger = \sum_k \prod_\rho C_{m_\rho^j - m_\rho^k}^\dagger(\rho) C_{m_\rho^i - m_\rho^k}(\rho) = \sum_k C_{j-k}^\dagger C_{i-k} \ , \tag{A13}$$

as was required.

Finally we note that theorem (A2) may be repeatedly applied to products of arbitrarily many configuration operators. As an application we prove Eq. (4.18) from the definition (4.13). We have

$$\langle \Phi | e^{S''} C_i C_l^\dagger C_m^\dagger | \Phi \rangle = \sum_n \langle \Phi | e^{S''} C_{l-n}^\dagger C_{i-n} C_m^\dagger | \Phi \rangle$$
$$= \sum_n \langle \Phi | e^{S''} C_{l-n}^\dagger C_{m-(i-n)}^\dagger | \Phi \rangle \ . \tag{A14}$$

Redefining $l \to l+n$, $m \to m+(i-n)$, we get from (4.13)

$$L_{jk}^i = \sum_{l,m,n} \langle \Phi | e^{S''} C_l^\dagger C_m^\dagger | \Phi \rangle \langle \Phi | e^{-S''} C_l C_n C_j^\dagger | \Phi \rangle \langle \Phi | e^{-S''} C_m C_{(i-n)} C_k^\dagger | \Phi \rangle$$
$$= \sum_{l,m,n} \langle \Phi | e^{S''} C_l^\dagger C_m^\dagger | \Phi \rangle \langle \Phi | e^{-S''} C_l C_{j-n}^\dagger | \Phi \rangle \langle \Phi | e^{-S''} C_m C_{k-(i-n)}^\dagger | \Phi \rangle$$
$$= \sum_n L_{j-n,k-(i-n)} \ , \tag{A15}$$

according to the definition (4.8) of L_{ij}. This completes the proof of Eq. (4.18).

APPENDIX B: MATRIX ELEMENTS AND RECURSION FORMULA FOR THE AVERAGE-VALUE FUNCTIONAL

Here we shall derive the explicit formal expression for the matrix elements of the average-value functional for an arbitrary operator. On the basis of Eqs. (3.25)–(3.29) one obviously can expand

$$\langle A \rangle = \sum_{m,n} \frac{1}{m!n!} \langle \Phi | [S'', [S'', \ldots, [\ldots [[A,S],S], \ldots, S] \ldots]] | \Phi \rangle \ , \tag{B1}$$

wherein the amplitude S'' is repeated m times, and the amplitude S is repeated n times. On the other hand, the defining equation (3.31) for the matrix elements directly gives

$$\langle i_1 \cdots i_m | A | j_1 \cdots j_n \rangle = \frac{\delta^m}{\delta\tilde{\sigma}_{i_1} \cdots \delta\tilde{\sigma}_{i_m}} \frac{\delta^n}{\delta\sigma_{j_1} \cdots \delta\sigma_{j_n}} \langle A \rangle |_{\sigma=\tilde{\sigma}=0} \ . \tag{B2}$$

We shall use this definition together with (B1) where now S and S'' must be expressed as functionals of σ and $\tilde{\sigma}$.

We shorten the notation by defining

$$S_{(kl\cdots)}^{(ij\cdots)} \equiv \frac{\delta}{\delta\tilde{\sigma}_i} \frac{\delta}{\delta\tilde{\sigma}_j} \cdots \frac{\delta}{\delta\sigma_k} \frac{\delta}{\delta\sigma_l} \cdots S \ , \tag{B3}$$

and use Eqs. (3.11), (3.21), and an equation analogous to (3.22) to obtain, at the point $\sigma=\tilde{\sigma}=0$,

$$S_{(j)} = C_j^\dagger \ , \tag{B4}$$

$$S_{(j)}^{(i_1 \cdots i_n)} = (-1)^n C_{j-i_1-\cdots-i_n}^\dagger \ ; \tag{B5}$$

all the other derivatives of S being zero. In the same way one gets at the points $\sigma=\tilde{\sigma}=0$

$$S''^{(i)} = C_i \ , \tag{B6}$$

other derivatives of S'' being zero.

We apply these results to the intermediate expression

$$\langle i_1 \cdots i_m | A | j_1 \cdots j_n \rangle = \frac{\delta^m}{\delta\tilde{\sigma}_{i_1} \cdots \delta\tilde{\sigma}_{i_m}} \sum_M \frac{1}{M!} \langle \Phi | [S'', [S'', \ldots, [\cdots [[A, S_{(j_1)}], S_{(j_2)}], \ldots, S_{(j_n)}] \cdots]] | \Phi \rangle \ , \tag{B7}$$

where the factor S'' appears M times and where now the limit $\sigma=\tilde{\sigma}=0$ is not yet taken. The m derivatives with respect to the amplitudes $\tilde{\sigma}_i$ must be distributed in all possible permutations among the amplitudes S'' and $S_{(j)}$ in (B7). The final outcome can be cast in the form

$$\langle i_1 \cdots i_m | A | j_1 \cdots j_n \rangle$$
$$= \sum_{m_1=0}^{m} \cdots \sum_{m_n=0}^{m} \sum_{P\{i\}} (-1)^{m_1+\cdots m_n} \frac{1}{M!}$$
$$\times \langle \Phi | [C_{k_1^n+1}, [C_{k_2^n+1}, [\ldots, [C_{k_M^n+1}, [\cdots [[A, C_{j_1-I_1}^\dagger], C_{j_2-I_2}^\dagger], \ldots, C_{j_n-I_n}^\dagger]] \cdots]]] | \Phi \rangle, \tag{B8}$$

where $P\{i\}$ denotes permutations over the set $\{i\}$, M is the integer number

$$M=m-m_1-m_2-\ldots-m_n\geqq 0\ , \tag{B9}$$

and I_ν denote the index sums

$$\begin{aligned} I_1&=k_1^1+\cdots+k_{m_1}^1\ ,\\ &\vdots\\ I_n&=k_1^n+\cdots+k_{m_n}^n\ , \end{aligned} \tag{B10}$$

and the index set $\{k_\nu^\mu \mid \mu=1,\ldots,n+1;\ \nu=1,\ldots,m_\mu\}$ (with $m_{n+1}\equiv M$) is a permutation of the set $(i_1,\ldots,i_m)$. An index sum I_ν may also be an empty set.

It is obvious that the matrix element (B2) is symmetric with respect to internal permutations of the indices $\{i\}$ or $\{j\}$. This is compatible with the fact that expressions of the form

$$f_{12\cdots n}=[\cdots[[A,K_1],K_2],\ldots,K_n] \tag{B11}$$

are symmetric in the indices $12\cdots n$, if the operators $\{K_i\}$ form a commuting algebra.

Formula (4.16) in Sec. IV gives an identity between the functional derivatives of an average value. It can be recast in the form of a condition on the matrix elements of the operator. By using the defining equation (3.31) we readily derive the following recursion formula:

$$\begin{aligned} {}^{m+1}\langle i+j,i_1\cdots i_m \mid A \mid j_1\cdots j_n\rangle^n &= {}^{m+2}\langle i,j,i_1\cdots i_m \mid A \mid j_1\cdots j_n\rangle^n\\ &+\sum_{l=1}^{n} {}^{m+1}\langle j,i_1\cdots i_m \mid A \mid j_1\ldots,(j_l-i),\ldots j_n\rangle^n\\ &+\sum_{l=1}^{n} {}^{m+1}\langle i,i_1\cdots i_m \mid A \mid j_1\ldots,(j_l-j),\ldots j_n\rangle^n\\ &+\sum_{k=1}^{n}\sum_{\substack{l=1\\(l\neq k)}}^{n} {}^{m}\langle i_1\cdots i_m \mid A \mid j_1\ldots,(j_k-i),\ldots,(j_l-j),\ldots j_n\rangle^n\ , \end{aligned} \tag{B12}$$

where the superscripts on the bra and ket states are an added reminder of the number of configuration indices in the states. This recursion equation is derivable also from the explicit expression (B8).

[1]J. Hubbard, Proc. R. Soc. London, Ser. A **240**, 539 (1957).

[2]F. Coester, Nucl. Phys. **7**, 421 (1958).

[3]F. Coester and H. Kümmel, Nucl. Phys. **17**, 477 (1960).

[4]H. Kümmel, K. H. Lührmann, and J. G. Zabolitzky, Phys. Rep. **36C**, 1 (1978).

[5]V. Kvasnička, V. Laurinc, and S. Biskupič, Phys. Rep. **90C**, 160 (1982).

[6]H. Kümmel, in *Nucleon-Nucleon Interaction and Nuclear Many-Body Problems,* edited by S. S. Wu and T. T. S. Kuo (World Scientific, Singapore, 1984), p. 46.

[7]J. Čížek, J. Chem. Phys. **45**, 4256 (1966); J Paldus, J. Čížek, and I. Shavitt, Phys. Rev. A **5**, 50 (1972); J. Paldus, J. Čížek, M. Saute, and A. Laforgue, *ibid.* **17**, 805 (1978).

[8]I. Lindgren, Int. J. Quantum Chem. Symp. **12**, 33 (1978).

[9]K. Szalewicz, J. G. Zabolitzky, B. Jeziorski, and H. J. Monkhorst, J. Chem. Phys. **81**, 2723 (1984).

[10]R. J. Bartlett and G. D. Purvis, Int. J. Quantum Chem. **14**, 561 (1978); G. D. Purvis and R. J. Bartlett, J. Chem. Phys. **76**, 1910 (1982); W. D. Laidig, G. D. Purvis, and R. J. Bartlett, J. Phys. Chem. **89**, 2161 (1985); H. Sekino and R. J. Bartlett, J. Chem. Phys. **84**, 2726 (1986).

[11]R. F. Bishop and K. H. Lührmann, Phys. Rev. B **17**, 3757 (1978); **26**, 5523 (1982).

[12]J. Arponen and E. Pajanne, J. Phys. C **15**, 2665 (1982); **15**, 2683 (1982).

[13]K. Emrich and J. G. Zabolitzky, Phys. Rev. B **30**, 2049 (1984).

[14]C. S. Hsue, H. Kümmel, and P. Ueberholz, Phys. Rev. D **32**, 1435 (1985).

[15]M. Altenbokum and H. Kümmel, Phys. Rev. D **32**, 2014 (1985).

[16]U. Kaulfuss, Phys. Rev. D **32**, 1421 (1985).

[17]R. K. Nesbet, Phys. Rev. **109**, 1632 (1958).

[18]H. Primas, in *Modern Quantum Chemistry,* edited by O. Sinanoglu (Academic, New York, 1965), Vol. II, p. 45.

[19]R. J. Bartlett and G. D. Purvis, Phys. Scr. **21**, 255 (1980).

[20]K. H. Lührmann, Ann. Phys. (NY) **103**, 253 (1977).

[21]K. Emrich, Nucl. Phys. **A351**, 379 (1981); **A351**, 397 (1981).

[22]R. Offermann, W. Ey, and H. Kümmel, Nucl. Phys. **A273**, 349 (1976); R. Offermann, Nucl. Phys. **A273**, 368 (1976).

[23]L. Z. Stolarczyk and H. J. Monkhorst, Phys. Rev. A **32**, 725 (1985); **32**, 743 (1985).

[24]R. F. Bishop, in *Nucleon-Nucleon Interaction and Nuclear Many-Body Problems,* edited by S. S. Wu and T. T. S. Kuo (World Scientific, Singapore, 1984), p. 604.

[25]R. F. Bishop, in *Recent Progress in Many-Body Theories,* edited by H. Kümmel and M. L. Ristig (Springer-Verlag, Berlin, 1984), p. 310.

[26]H. J. Monkhorst, Int. J. Quantum Chem. Symp. **11**, 421 (1977); E. Dalgaard and H. J. Monkhorst, Phys. Rev. A **28**, 1217 (1983).
[27]J. Čížek, Adv. Chem. Phys. **14**, 35 (1969); M. Fink, Nucl. Phys. **A221**, 163 (1974).
[28]K. H. Lührmann (unpublished); H. G. Kümmel, Int. J. Quantum Chem. **24**, 79 (1983).
[29]D. J. Thouless, *The Quantum Mechanics of Many-Body Systems* (Academic, New York, 1961).
[30]J. Arponen, Ann. Phys. (NY) **151**, 311 (1983).
[31]J. Arponen and J. Rantakivi, Nucl. Phys. **A407**, 141 (1983).
[32]J. Arponen, J. Phys. G **8**, L129 (1982).
[33]S. Pal, Phys. Rev. A **33**, 2240 (1986); **34**, 2682 (1986).
[34]J. Arponen, R. F. Bishop, and E. Pajanne, following paper, Phys. Rev. A **36**, 2539 (1987).
[35]H. J. Lipkin, N, Meshkov, and A. J. Glick, Nucl. Phys. **62**, 188 (1965); **62**, 199 (1965); **62**, 211 (1965).
[36]F. Coester, in Vol. XI-B of *Lectures in Theoretical Physics,* edited by K. T. Mahanthappa and W. E. Brittin (Gordon & Breach, New York, 1969).
[37]T. Holstein and H. Primakoff, Phys. Rev. **58**, 1098 (1940).
[38]F. J. Dyson, Phys. Rev. **102**, 1217 (1956); **102**, 1230 (1956).
[39]J. Schwinger, in *Quantum Theory of Angular Momentum,* edited by L. C. Biedenharn and H. van Dam (Academic, New York, 1965), p. 229.
[40]T. Marumori, M. Yamamura, and A. Tokunaga, Prog. Theor. Phys. **31**, 1009 (1964).
[41]D. Janssen, F. Dönau, S. Frauendorf, and R. V. Jolos, Nucl. Phys. **A172**, 145 (1971).
[42]J. Arponen and E. Pajanne, Ann. Phys. (NY) **91**, 450 (1975).
[43]P. Garbaczewski, Phys. Rep. **36C**, 65 (1978).
[44]R. J. Glauber, Phys. Rev. Lett. **10**, 84 (1963); Phys. Rev. **130**, 2529 (1963); **131**, 2766 (1963).
[45]J. R. Klauder and B.-S. Skagerstam, *Coherent States—Applications in Physics and Mathematical Physics* (World Scientific, Singapore, 1985).
[46]R. Abraham and J. E. Marsden, *Foundations of Mechanics,* 2nd ed. (Benjamin, Reading, Mass., 1978).
[47]P. Hohenberg and W. Kohn, Phys. Rev. **136**, B864 (1964).
[48]W. Kohn and L. J. Sham, Phys. Rev. **140**, A1133 (1965).
[49]U. Kaulfuss and M. Altenbokum, Phys. Rev. D **35**, 609 (1987) and references therein.
[50]I. S. Gradshteyn and I. M. Ryzhik, *Table of Intergrals, Series and Products* (Academic, New York, 1965).