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Extended coupled-cluster method. II. Excited states and generalized random-phase approximation

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This article gives a discussion of the application of the extended coupled-cluster method (ECCM) to the excited states of a general quantum many-body system. The direct eigenvalue equations for the excitation amplitudes of both the ket and the bra eigenstates are derived in the biorthogonal basis obtained by a double similarity transformation. The equations correspond to the diagonalization of a matrix involving second-order functional derivatives of the average-value functional for the Hamiltonian with respect to the basic ECCM amplitudes. The same excitation spectrum is obtained by considering small oscillations around the equilibrium. The problem with its associated effective Hamiltonian has the structure of a generalized random-phase approximation. By diagonalizing the effective Hamiltonian we perform a canonical or symplectomorphic coordinate transformation into normal coordinates in the symplectic ECCM phase space. In this coordinate system the exact average-value functional for the Hamiltonian has a structure analogous to that of classical lattice dynamics or the phenomenological Ginzburg-Landau theory. At all stages the method satisfies the property of quantum locality, which in real space shows up as a definite quasilocality. Due to this property the method allows, for example, the treatment of mesonlike excitations in the presence of topological objects or in other symmetry-broken equilibrium states.

I. INTRODUCTION

In an earlier paper[1] (hereafter referred to as I) we demonstrated how the extended coupled-cluster method[2] (ECCM) could be used to give a very convenient parametrization of the Hilbert space appropriate to the general quantum-mechanical many-body problem. Indeed the formalism is applicable to any system for which a Schrödinger dynamics is defined. We showed in I how the ECCM equations of motion could be derived both from a dynamic variational principle for a suitably parametrized action functional and, more directly, from the ground-state Schrödinger equation itself. We demonstrated rather explicitly how the double similarity transformation which underpins and characterizes the ECCM leads to several desirable features.

In the first place, the expectation value for an arbitrary operator is expressed entirely in terms of the linked-cluster amplitudes $\{\sigma_i,\tilde{\sigma}_i\}$ that completely characterize the ECCM formulation. Furthermore, these expectation values $\langle A \rangle$ for an arbitrary operator A are completely compatible with the energy expectation value in the usual Thouless[3] sense that the former can be obtained from the usual Goldstone diagrams for the energy by replacing each interaction in turn by the operator A.

Secondly, we showed how the basic amplitudes $\{\sigma_i,\tilde{\sigma}_i\}$ could be viewed as a set of quasilocal classical fields, due to the maximal connectivity feature built into the ECCM. By quasilocality here, we mean that each of the amplitudes which between them completely characterize the theory obeys the cluster property in the usual sense of becoming zero in the limit that any one particle or group of particles contained in the configuration-space index i becomes far removed from the remainder. Further, we showed how the quantum many-body theory could be mapped exactly onto a classical Hamiltonian mechanics for the many-body, classical (c-number) configuration-space amplitudes $\{\sigma_i,\tilde{\sigma}_i\}$. This mapping was seen to arise from an underlying one-to-one correspondence between the set of commutators in the original quantal Hilbert space and a set of suitably defined generalized classical Poisson brackets.

Thirdly, we showed how the ECCM can also be interpreted as an exact generalized mean-field theory formulation of the original quantum many-body problem. This interpretation was seen to be intimately linked with the realization that the ECCM could also be viewed as an exact bosonization procedure in which the ECCM states could be associated in a one-to-one fashion with a set of generalized coherent states in some suitably defined boson space. This ECCM bosonization procedure differs from other such procedures by having taken the usual motivation for any bosonization scheme to its logical conclusion—namely, that the resultant generalized

coherent boson fields are classical c-number fields with only classical (nonlinear) interactions between them. This feature of being able to reinterpret the ECCM as an exact generalized mean-field theory was reinforced by the observation that the ECCM bosonization maps commutators of operators in the original Hilbert space only into the tree-level pieces of the corresponding commutators of the respective mapped operators in their boson image space. The tree level of a commutator is here defined to be a restriction only to such contractions which do not result in closed loops.

The entire formulation of the ECCM presented in I was based on a parametrization of the ground state of the many-body system, and its dynamical evolution. However, the exact generalized mean-field-theory aspect of the ECCM discussed above led us inexorably to the view that the basic field amplitudes $\{\sigma_i,\tilde{\sigma}_i\}$ could in some sense be viewed as a set of collective coordinates for the system. It is one of the purposes of the present paper to elaborate this feature further. With this viewpoint in mind it is natural to attempt an ECCM formulation of the excited states as well as for the ground state. There are basically two distinct ways that we may do this, and in the present paper we develop both. From the deep connections between them we are thereby able to shed further light on the interpretation of our basic field variables as collective coordinates. After some preliminary discussion in Sec. II, the main aim of which is to recapitulate and gather together the most important results from I that we need for present purposes, we discuss these two methods in turn.

In Sec. III we describe what is perhaps the most direct further extension to excited states of the ground-state ECCM. This direct approach is based on the relationship between the ECCM and the normal coupled-cluster method (CCM) or exp(S) method of Coester and Kümmel.[4,5] The normal CCM was originally invented as a parametrization of a nondegenerate quantum-mechanical ground state, just as was the ECCM.[2] The normal CCM was later further developed by Emrich[6] to describe excited states; and the previous ground-state ECCM is now also directly generalized to excited states in Sec. III by analogy with the underlying ideas of Emrich. We show that the excitation energies and the configuration-space amplitudes which parametrize the excited-state wave functions are thereby obtained in the form of a set of linear eigenvalue equations. We show explicitly how their solution may then be obtained by diagonalizing a certain effective Hamiltonian matrix. Its elements are uniquely specified in terms of the second-order functional derivatives with respect to the basic ground-state field amplitudes $\{\sigma_i,\tilde{\sigma}_i\}$ of the expectation value $\langle H\rangle$ of the Hamiltonian, evaluated in the stationary (equilibrium) ground-state configuration.

In Sec. IV this previous direct approach is augmented by considering the dynamics of the basic field amplitudes $\sigma_i(t)=\sigma_i^0+\delta\sigma_i(t)$, $\tilde{\sigma}_i(t)=\tilde{\sigma}_i^{\,0}+\delta\tilde{\sigma}_i(t)$ when they are restricted to small perturbations $\delta\sigma_i,\delta\tilde{\sigma}_i$ away from their stable ground-state equilibrium values $\sigma_i^0,\tilde{\sigma}_i^{\,0}$. In this way, the collective eigenmodes are found by linearizing the general equations of motion given in I. Thus the energy expectation value $\langle H\rangle$ is expanded in powers of the deviations $\delta\sigma_i,\delta\tilde{\sigma}_i$ around the ground-state values, and the method again reduces to a diagonalization of the second-order terms in the expansion.

We demonstrate that there is a one-to-one correspondence between the excited states obtained in Sec. III and the collective eigenmodes obtained in Sec. IV for small oscillations about the ground-state equilibrium. We also demonstrate how the effective Hamiltonian approach of Sec. IV may be viewed as an exact generalization of the well-known random-phase approximation (RPA) of Bohm and Pines.[7] Just as the usual RPA may be viewed as the small-perturbation dynamics of the (classical) mean fields about their equilibrium values, so we show that our exact generalized RPA may, in complete analogy, be viewed as the small-perturbation dynamics of our generalized amplitudes $\sigma_i,\tilde{\sigma}_i$ about their equilibrium values. This feature makes very precise their previous interpretation as exact generalized (classical) mean fields in the many-body configuration space.

In Sec. V we calculate explicitly the collective eigenmodes of the effective Hamiltonian that was obtained from the average value $\langle H\rangle$ of the Hamiltonian by expanding in powers of the deviations $\delta\sigma_i,\delta\tilde{\sigma}_i$ around the stable configuration $\sigma_i^0,\tilde{\sigma}_i^{\,0}$, and by retaining in this expansion only terms up to second order in $\delta\sigma_i,\delta\tilde{\sigma}_i$. We can diagonalize this effective Hamiltonian by choosing new coordinates $\psi(\varepsilon),\tilde{\psi}(\varepsilon)$ in the ECCM phase space. These normal-mode amplitudes $\psi(\varepsilon)$ and $\tilde{\psi}(\varepsilon)$ are linear functions of the deviations $\delta\sigma_i,\delta\tilde{\sigma}_i$ with coefficients given by the eigenvectors of the dynamical matrix of Sec. IV. The resulting quadratic diagonal effective Hamiltonian gives correctly the linear-response limit for the system. To describe larger perturbations, one clearly has to include in the expansion of $\langle H\rangle$ terms of higher order in $\psi(\varepsilon)$ and $\tilde{\psi}(\varepsilon)$, which would then lead to a theory that resembles the Ginzubrg-Landau type of phenomenological approach.

II. PRELIMINARY REMARKS

The idea of the ECCM parametrization is based on the use of a double-similarity transformation, and one defines accordingly the transformed Hamiltonian $\hat{H}$ to be

$$\hat{H}=e^{S''}e^{-S}He^{S}e^{-S''}\,, \tag{2.1}$$

where S is composed of creation and S'' of destruction operators, respectively, with respect to some appropriate state $|\Phi\rangle$ defined below. The ket and bra ground states of the system are

$$|\Psi_0\rangle=e^{S}e^{-S''}|\Phi\rangle=e^{S}|\Phi\rangle\,, \tag{2.2a}$$

$$\langle\Psi_0'|=\langle\Phi|e^{S''}e^{-S}\,, \tag{2.2b}$$

where $|\Phi\rangle$ is the model state. It is immediately clear that the ground states are normalized, $\langle\Psi_0'|\Psi_0\rangle=1$. Likewise it is obvious that the extended formulation is not manifestly Hermitian. This derives from the fact that the double-similarity transformations, which generate the ket and bra ground states in Eqs. (2.2a) and (2.2b), are not unitary. The ECCM formalism leads rather to a biorthogonal formulation of the many-body problem.

Hence in this general case we define the ground-state eigenvalue problems both for the ket and the bra eigenstates in a unified way,

$$H\,|\Psi_0\rangle=E_0\,|\Psi_0\rangle\rightarrow\hat{H}\,|\Phi\rangle=E_0\,|\Phi\rangle\ , \tag{2.3a}$$

$$\langle\Psi_0'|\,H=\langle\Psi_0'|\,E_0\rightarrow\langle\Phi|\,\hat{H}=\langle\Phi|\,E_0\ . \tag{2.3b}$$

The amplitudes S and S'' can be written in terms of normalized configuration creation and destruction operators $C_i^\dagger$ and C_i as follows:

$$S=\sum_i{}'\,S_iC_i^\dagger\ , \tag{2.4a}$$

$$S''=\sum_i{}'\,S_i''C_i\ , \tag{2.4b}$$

where the precise meaning of the configuration-space index $\{i\}$ is discussed in detail in I, and where the primed sum means that at least one particle is created or destroyed ($i\neq0$). As was stated in I, the most practical parametrization is achieved by changing from the set $\{S_i,S_i''\}$ to a set of new amplitudes $\{\sigma_i,\bar{\sigma}_i\}$ which are defined as

$$\sigma_i=\langle\Phi|\,C_ie^{S''}S\,|\Phi\rangle\ , \tag{2.5a}$$

$$\bar{\sigma}_i=S_i''\ . \tag{2.5b}$$

The average value of the Hamiltonian

$$\langle H\rangle=\langle\Psi_0'|\,H\,|\Psi_0\rangle=\langle\Phi|\,\hat{H}\,|\Phi\rangle \tag{2.6}$$

is now a functional of the amplitudes $\sigma,\bar{\sigma}$, i.e., $\langle H\rangle=\bar{H}[\sigma,\bar{\sigma}]$. This functional is of particular importance, because it determines the dynamics of the amplitudes σ and $\bar{\sigma}$ and their ground-state equilibrium values. As was shown in I, e.g., with the help of a dynamical variational principle, the equations of motion are

$$i\dot{\sigma}_i=\frac{\delta\langle H\rangle}{\delta\bar{\sigma}_i}\bigg|_\sigma\ , \tag{2.7a}$$

$$i\dot{\bar{\sigma}}_i=-\frac{\delta\langle H\rangle}{\delta\sigma_i}\bigg|_{\bar{\sigma}}\ . \tag{2.7b}$$

An important result derived in I is that various matrix elements involving the double-similarity transform $\hat{A}$ of a general operator A, defined analogously to Eq. (2.1), can be related to the functional derivatives with respect to the basic amplitudes $\sigma,\bar{\sigma}$ of its average-value functional $\langle A\rangle$. Hence we have devised a method that allows the evaluation of average values of arbitrary operator products. Especially useful for present purposes will be matrix elements such as

$$\langle\Phi|\,C_i\hat{A}C_j^\dagger\,|\Phi\rangle=\langle A\rangle\delta(i,j)+\frac{\delta\langle A\rangle}{\delta\sigma_{j-i}}+\sum_k{}'\frac{\delta\langle A\rangle}{\delta\sigma_k}\sum_l{}'\sigma_{k+l}L_{lj}^i+\sum_k{}'\frac{\delta\langle A\rangle}{\delta\bar{\sigma}_k}L_{kj}^i+\sum_k{}'\frac{\delta^2\langle A\rangle}{\delta\sigma_j\delta\sigma_k}\sigma_{k+i}+\frac{\delta^2\langle A\rangle}{\delta\bar{\sigma}_i\delta\sigma_j}\ , \quad i\neq0\neq j \tag{2.8}$$

where the coefficient L_{jk}^i is defined as

$$L_{jk}^i=L_{kj}^i=\sum_l\sum_m\omega_{(l+m)-i}\bar{\omega}_{j-l}\bar{\omega}_{k-m},\quad L_{jk}^0\equiv L_{jk}\ . \tag{2.9}$$

For the detailed definitions of how to add and subtract configuration indices, we refer the reader to I. The functionals ω_i and $\bar{\omega}_i$ are

$$\omega_i=\omega_i[\bar{\sigma}]\equiv\langle\Phi|\,e^{S''}C_i^\dagger\,|\Phi\rangle\ , \tag{2.10a}$$

$$\bar{\omega}_i=\bar{\omega}_i[\bar{\sigma}]\equiv\langle\Phi|\,e^{-S''}C_i^\dagger\,|\Phi\rangle\ . \tag{2.10b}$$

In the following study of excited states, we have frequent need of the identity between the first- and second-order functional derivatives of the average-value functional $\langle A\rangle$, proven in I,

$$\frac{\delta\langle A\rangle}{\delta\bar{\sigma}_{i+j}}=\frac{\delta^2\langle A\rangle}{\delta\bar{\sigma}_i\delta\bar{\sigma}_j}+\sum_k{}'\left[\sigma_{i+k}\frac{\delta^2\langle A\rangle}{\delta\sigma_k\delta\bar{\sigma}_j}+\frac{\delta^2\langle A\rangle}{\delta\bar{\sigma}_i\delta\sigma_k}\sigma_{k+j}\right]+\sum_k{}'\sum_l{}'\sigma_{i+k}\frac{\delta^2\langle A\rangle}{\delta\sigma_k\delta\sigma_l}\sigma_{l+j}\ . \tag{2.11}$$

III. DESCRIPTION OF EXCITED STATES

A. Ket eigenstates

The Hubbard-Coester theorem[4,8] concerning the linked-cluster nature of the operator S in the exp$S$ parametrization of the ground state can be in principle extended also to the excited states. For each excited state, then, the model state $|\Phi\rangle$ should be taken as an excited (noninteracting) model state, and the creation operators $\{C_i^\dagger\}$ should be redefined with respect to this excited model state. This scheme has not, however, been developed further mainly because it is cumbersome and not without certain dangers due to strong assumptions of adiabaticity in the behavior of the excited states as the interaction is switched on.

From the point of view of finding suitable parametrizations for the excited states, the problem has therefore remained more open, and several different approaches have been developed. In few-body physics, notably in quantum chemistry, various formulations of the open-shell or degenerate perturbation theory have been suggested and applied. For example, it has been rigorously shown[9] that the degenerate perturbation theory also leads to definite linked-cluster or exp$S$ structures, which differ

from the ground-state formalism mainly due to the appearance of folded diagrams.[10] On the other hand, starting from CCM there have appeared reformulations and applications to the open-shell problems by various authors.[11]

Typical of these methods is the division of single-particle states into the subspaces of core, model (or valence) and particles states.[10,11] Such a division is not usually very natural for such extended systems as quantum liquids. Emrich[6] therefore suggested an alternative method, which avoids this artificial division and is more closely related to the original Coester-Kümmel approach. The present treatment is based on the ideas of Emrich (see also the discussion in Ref. 12), and generalizes them to the ECCM formalism.

Consider the eigenvalue problem

$$H\,|\Psi_\lambda\rangle=(E_0+\varepsilon_\lambda)\,|\Psi_\lambda\rangle\ , \tag{3.1}$$

where ε_λ is the (positive) excitation energy. In the similarity-transformed basis we write the analogous eigenvalue equation for the transformed operator $\hat{H}$,

$$\hat{H}\,|\chi_\lambda\rangle=(E_0+\varepsilon_\lambda)\,|\chi_\lambda\rangle\ ; \tag{3.2}$$

hence the connection is

$$|\Psi_\lambda\rangle=e^{S}e^{-S''}\,|\chi_\lambda\rangle\ . \tag{3.3}$$

A convenient and sufficiently general parametrization for $|\chi_\lambda\rangle$ is to express it in terms of an excitation (creation) amplitude X^λ as follows:

$$\hat{H}X^\lambda\,|\Phi\rangle=(E_0+\varepsilon_\lambda)X^\lambda\,|\Phi\rangle\ . \tag{3.4}$$

Due to equation (2.3a) this further implies

$$[\hat{H},X^\lambda]\,|\Phi\rangle=\varepsilon_\lambda X^\lambda\,|\Phi\rangle\ . \tag{3.5}$$

We can express the eigenvalue equation in terms of matrix elements by introducing the vector coefficients

$$X_i^\lambda\equiv\langle\Phi\,|\,C_iX^\lambda\,|\,\Phi\rangle\ . \tag{3.6}$$

It is immediately obvious by projecting Eq. (3.5) onto $\langle\Phi|$ that $X_0^\lambda=0$, provided $\varepsilon_\lambda\neq0$. As for the matrix elements of $\hat{H}$ use must be made of Eq. (2.8) and of the fact that at the stationary point the first-order functional derivatives of $\langle H\rangle$ vanish. For simplicity let us denote

$$E_{ij}\equiv\frac{\delta^2\langle H\rangle}{\delta\tilde{\sigma}_i\delta\sigma_j}\ , \tag{3.7}$$

$$F_{ij}\equiv\frac{\delta^2\langle H\rangle}{\delta\sigma_i\delta\sigma_j}\ , \tag{3.8}$$

$$\tilde{F}_{ij}\equiv\frac{\delta^2\langle H\rangle}{\delta\tilde{\sigma}_i\delta\tilde{\sigma}_j}\ . \tag{3.9}$$

Equation (2.8) gives at the stationary point, for $i\neq0\neq j$,

$$\langle\Phi\,|\,C_i\hat{H}C_j^\dagger\,|\,\Phi\rangle=E_0\delta(i,j)+E_{ij}+\sum_k{}'\,\sigma_{i+k}F_{kj}\ , \tag{3.10}$$

and the eigenvalue equation for the ket state therefore becomes

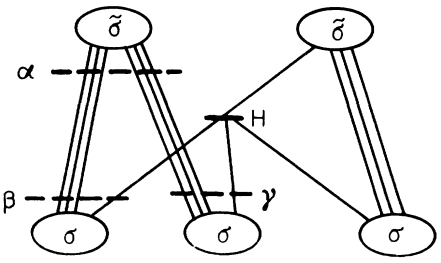

FIG. 1. Typical term in the expansion of the average value $\langle H\rangle\equiv\bar{H}[\sigma,\tilde{\sigma}]$. The small bar labeled H indicates the Hamiltonian vertex, and the lines between the amplitudes $\sigma,\tilde{\sigma}$ and H are single-particle contractions. The dashed lines labeled α, β, and γ are the cuts referred to in the text.

$$\sum_j{}'\left[E_{ij}+\sum_k{}'\,\sigma_{i+k}F_{kj}-\varepsilon_\lambda\delta(i,j)\right]X_j^\lambda=0,\quad i\neq0\ . \tag{3.11}$$

It is perhaps also useful to digress briefly to consider the connectivity properties of the basic second-order functional derivatives E_{ij}, F_{ij}, and $\tilde{F}_{ij}$ that now characterize our excited-state formalism. The connectivity properties of $\langle H\rangle$ have already been given in considerable detail in I, particularly in Eqs. (3.30) and (3.31) and the surrounding discussion. Basically, we described in I how a double (or definite) linking structure arises such that in the expansion of $\langle H\rangle\equiv\bar{H}[\sigma,\tilde{\sigma}]$, only such terms occur where each $\tilde{\sigma}_i$ amplitude is linked to at least two different amplitudes σ_j, unless the $\tilde{\sigma}_i$ amplitude is linked directly to the operator H. A typical term in the expansion of $\langle H\rangle$ from Eq. (3.31) of I is shown in Fig. 1. It is clear that cutting off any number of $\tilde{\sigma}$ amplitudes (such as indicated for example by the cut α in Fig. 1 to remove a single $\tilde{\sigma}$ amplitude) leaves the remaining diagram fully connected. Thus all functional derivatives $\delta^n\langle H\rangle/\delta\tilde{\sigma}_{i_1}\cdots\delta\tilde{\sigma}_{i_n}$ are connected, for all values of n. In particular, the amplitude $\tilde{F}_{ij}$ is connected. Similarly, the removal of a single σ amplitude (such as indicated by the cuts labeled β or γ in Fig. 1) shows that $\delta\langle H\rangle/\delta\sigma_i$ is connected. However, both E_{ij} and F_{ij} may be disconnected. For example, in the case of E_{ij}, the cuts

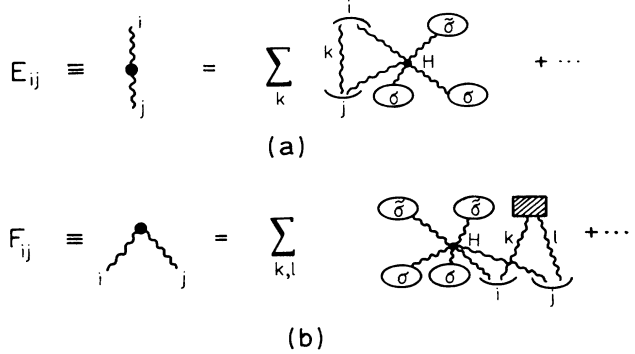

FIG. 2. Diagrammatic representation of the connectivity structure of (a) E_{ij}, and (b) F_{ij}. The shaded box indicates the function L_{kl} defined in Eq. (2.9), and the wavy lines denote many-body configurations.

α and β in Fig. 1 leave the remaining diagram disconnected; and similarly for F_{ij} cuts at β and γ also leave it disconnected. One can, by such considerations, define fully connected pieces E^c_{ij} and F^c_{ij} in terms of which the general E_{ij} and F_{ij} may respectively be expressed. The resulting expressions are easily obtained diagrammatically as in Fig. 2, the explicit algebraic form of which we do not give.

B. Bra eigenstates

Following the procedure introduced in the previous chapter we write the eigenvalue equation in the form

$$\langle \Phi \mid Y^\lambda \hat{H} = (E_0 + \varepsilon_\lambda) \langle \Phi \mid Y^\lambda \ , \tag{3.12}$$

in which the deexcitation amplitude Y^λ is composed of destruction operators only. The left eigenstate of the Hamiltonian H is then given by

$$\langle \Psi'_\lambda \mid = \langle \Phi \mid Y^\lambda e^{S''} e^{-S} \ . \tag{3.13}$$

In matrix form the coefficients Y^λ_i, defined as

$$Y^\lambda_i \equiv \langle \Phi \mid Y^\lambda C_i^\dagger \mid \Phi \rangle \ , \tag{3.14}$$

satisfy the eigenvalue equation

$$\sum_j{}' \, Y^\lambda_j \left[E_{ji} + \sum_k{}' \, \sigma_{j+k} F_{ki} - \varepsilon_\lambda \delta(i,j) \right] = 0 \ . \tag{3.15}$$

The right- and left-hand eigenvector equations (3.11) and (3.15) are represented pictorially in Figs. 3 and 4, respectively. We note also that $Y^\lambda_0 = \langle \Phi \mid Y^\lambda \mid \Phi \rangle = 0$, exactly as in the case of the ket eigenstates.

Just as in standard quantum mechanics we can further prove the orthogonality of the left and right eigenstates, because

$$\begin{aligned} \langle \Phi \mid Y^\lambda \hat{H} X^{\lambda'} \mid \Phi \rangle &= (E_0 + \varepsilon_\lambda) \langle \Phi \mid Y^\lambda X^{\lambda'} \mid \Phi \rangle \\ &= (E_0 + \varepsilon_{\lambda'}) \langle \Phi \mid Y^\lambda X^{\lambda'} \mid \Phi \rangle \ . \end{aligned} \tag{3.16}$$

If $\varepsilon_{\lambda'} \neq \varepsilon_\lambda$, the matrix element must be zero, and we therefore should be able to choose the normalization to satisfy

$$\langle \Phi \mid Y^\lambda X^{\lambda'} \mid \Phi \rangle = \delta_{\lambda,\lambda'} \ . \tag{3.17}$$

What we have achieved is a complete biorthonormal description of the spectrum of the Hamiltonian. The description takes into account, as fully as possible, the linked-cluster structure of the perturbative eigenvalue problem. Yet the coupled-cluster problem for the determination of S and S'' has to be solved only once, namely, for the ground state, just as in Emrich's theory.[6] The remaining problem consists of diagonalizing the matrix of

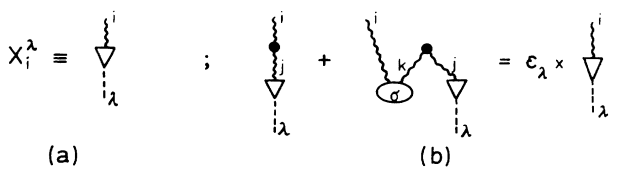

FIG. 3. Diagrammatic representation of (a) the excited ket-state amplitudes X^λ_i and (b) their eigenvalue equation (3.11).

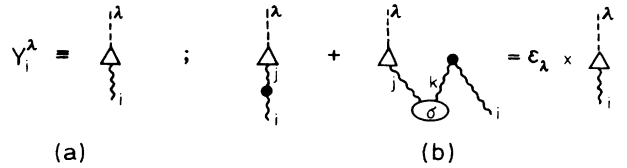

FIG. 4. Diagrammatic representation of (a) the excited bra-state amplitudes Y^λ_i and (b) their eigenvalue equation (3.15).

a certain effective Hamiltonian, composed of the second-order functional derivatives of the average value $\langle H \rangle$ at the stationary point. This problem is a linear homogeneous eigenvalue problem and of the same form for all excited states. The physical motivation behind this idea derives from the assumption that the interparticle correlations in (at least the important low-lying) excited states are essentially similar to those in the ground state, which is already accurately treated by the ground-state $\exp(S)$ transformation.[6] Therefore the excitation operators Y^λ, X^λ have the potentiality of being very simple.

IV. AN EFFECTIVE HAMILTONIAN APPROACH TO THE EIGENVALUE PROBLEM

The dynamics of small oscillations around the stationary point is governed by an effective Hamiltonian, which can be obtained by linearizing the equations of motion (2.7a) and (2.7b). Close to the stationary point the average value of the Hamiltonian, including terms up to second order, is

$$\begin{aligned} \bar{H}^{(2)} = E_0 + \sum_i{}' \sum_j{}' (& \delta\tilde{\sigma}_i E_{ij} \delta\sigma_j + \tfrac{1}{2} \delta\tilde{\sigma}_i \tilde{F}_{ij} \delta\tilde{\sigma}_j \\ & + \tfrac{1}{2} \delta\sigma_i F_{ij} \delta\sigma_j) \ . \end{aligned} \tag{4.1}$$

The equations of motion can then be written in block matrix form as

$$i \frac{d}{dt} \begin{bmatrix} \delta\sigma_j \\ \delta\tilde{\sigma}_j \end{bmatrix} = \sum_k{}' \begin{bmatrix} E_{jk} & \tilde{F}_{jk} \\ -F_{jk} & -E_{kj} \end{bmatrix} \begin{bmatrix} \delta\sigma_k \\ \delta\tilde{\sigma}_k \end{bmatrix} \ , \tag{4.2}$$

which introduces the effective Hamiltonian (or the dynamical matrix)

$$H_D \equiv \begin{bmatrix} E & \tilde{F} \\ -F & -E^T \end{bmatrix} \ . \tag{4.3}$$

We use the superscript T to denote the transpose of a matrix or a vector.

To find the eigenfrequencies of the oscillations we must solve the right-hand eigenvalue problem

$$H_D \begin{bmatrix} \xi(\varepsilon) \\ \eta(\varepsilon) \end{bmatrix} = \varepsilon \begin{bmatrix} \xi(\varepsilon) \\ \eta(\varepsilon) \end{bmatrix} \ , \tag{4.4}$$

or, equivalently, the left-hand eigenvalue problem

$$[\tilde{\xi}(\varepsilon)^T \ \ \tilde{\eta}(\varepsilon)^T] H_D = [\tilde{\xi}(\varepsilon)^T \ \ \tilde{\eta}(\varepsilon)^T] \varepsilon \ . \tag{4.5}$$

Due to the non-Hermiticity of H_D, the left vectors $\tilde{\xi}(\varepsilon), \tilde{\eta}(\varepsilon)$ bear no obvious relationship to the right vectors $\xi(\varepsilon), \eta(\varepsilon)$. Figures 5 and 6 give a pictorial representation

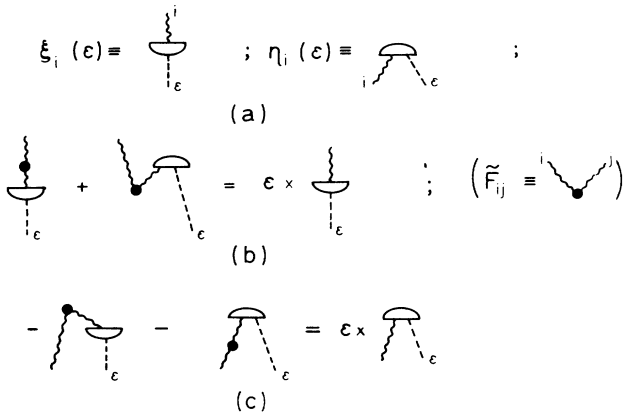

FIG. 5. Diagrammatic representation of (a) the right-hand eigenstates $\xi_i(\varepsilon)$ and $\eta_i(\varepsilon)$ for $\varepsilon>0$, and (b), (c) their respective coupled eigenvalue equations from Eq. (4.4).

of the eigenvalue equations (4.4) and (4.5), respectively.

A closer scrutiny of the dynamical matrix reveals that it is the product of an antisymmetric and a symmetric matrix,

$$H_D=\begin{bmatrix} 0 & I \\ -I & 0 \end{bmatrix}\begin{bmatrix} F & E^T \\ E & \tilde{F} \end{bmatrix}, \tag{4.6}$$

since F and $\tilde{F}$ are symmetric. Due to this fact the eigenvalues ε must appear in pairs $\pm\varepsilon$, and the characteristic polynomial is actually a function of ε^2 (see Refs. 13 and 14). By a few simple manipulations utilizing the symmetry of H_D we can also get from Eq. (4.4) the equivalent equation

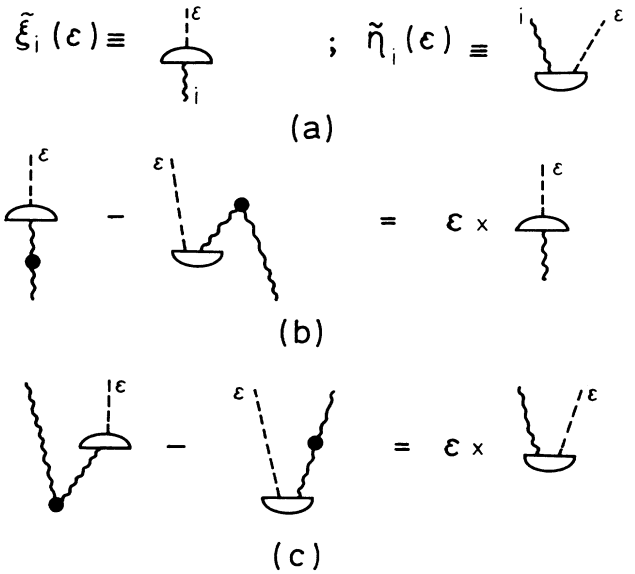

FIG. 6. Diagrammatic representation of (a) the left-hand eigenstates $\tilde{\xi}_i(\varepsilon)$ and $\tilde{\eta}_i(\varepsilon)$ for $\varepsilon>0$, and (b), (c) their respective coupled eigenvalue equations from Eq. (4.5).

$$[\eta(\varepsilon)^T \ -\xi(\varepsilon)^T]H_D=-\varepsilon[\eta(\varepsilon)^T \ -\xi(\varepsilon)^T], \tag{4.7}$$

which, by comparison with Eq. (4.5), actually relates the left and right eigenstates corresponding to opposite energies,

$$\begin{bmatrix} \tilde{\xi}(\varepsilon) \\ \tilde{\eta}(\varepsilon) \end{bmatrix}=\begin{bmatrix} \eta(-\varepsilon) \\ -\xi(-\varepsilon) \end{bmatrix}. \tag{4.8}$$

The equivalences expressed in Eq. (4.8) imply that the solutions of the right and left eigenvalue equations (4.4) and (4.5) may be restricted to positive eigenvalues $\varepsilon>0$ only. The corresponding negative-energy solutions then simply amount to permutations of the positive-energy solutions. This restriction to positive eigenvalues is implied in all our diagrams for the amplitudes ξ, η, $\tilde{\xi}$, and $\tilde{\eta}$.

The normalization of the eigenvectors can be chosen to satisfy

$$\begin{aligned}[\tilde{\xi}(\varepsilon)^T \ \tilde{\eta}(\varepsilon)^T]&\begin{bmatrix} \xi(\varepsilon') \\ \eta(\varepsilon') \end{bmatrix} \\ &=\sum_i{}'\{\tilde{\xi}_i(\varepsilon)\xi_i(\varepsilon')+\tilde{\eta}_i(\varepsilon)\eta_i(\varepsilon')\} \\ &=\sum_i{}'\{\eta_i(-\varepsilon)\xi_i(\varepsilon')-\xi_i(-\varepsilon)\eta_i(\varepsilon')\} \\ &=\delta_{\varepsilon,\varepsilon'}\mathrm{sgn}(\varepsilon)\,.\end{aligned} \tag{4.9}$$

The above analysis displays an obvious analogy to the well-known random-phase approximation (RPA) of Bohm and Pines.[7] In one form or other, the RPA has turned out to be a versatile approach to dynamical phenomena in many fields of physics. The great advantage of the RPA-type approximation scheme is its nonperturbative nature, which allows one to obtain ground-state or excitation energies that are nonanalytic functions of the coupling constant or indeed of any other coefficient appearing in the Hamiltonian.

The present ECCM formulation of the dynamics of small oscillations is thus a definite generalization of RPA, with two major differences. The indices i are configuration indices and involve, therefore, arbitrarily many single-particle degrees of freedom, whereas in ordinary RPA the indices i are restricted to single particles (or particle-hole pairs in the fermion case). The second difference is that the present formalism, if not truncated, is exact and not just an approximation.

There clearly must be a connection between the problem of eigenfrequencies of small oscillations and the ket and bra eigenvalue problems. The connection is established as follows.

The crucial factor is the identity (2.11). If applied to the Hamiltonian at the stationary point, where the first functional derivatives vanish, it yields the result

$$\tilde{F}+E\sigma+\sigma E^T+\sigma F\sigma=0\,. \tag{4.10}$$

Here we use an obvious matrix notation by defining $(\sigma)_{ij}\equiv\sigma_{i+j}$. If $\tilde{F}$ is solved from Eq. (4.10) and inserted into the right-hand eigenvalue equations (4.4), which due to the equivalences (4.8) actually constitute a complete set of eigenvalue equations for both signs of ε, one finds

$$(E-\varepsilon)\xi-(E\sigma+\sigma E^T+\sigma F\sigma)\eta=0\ , \tag{4.11a}$$

$$F\xi+(E^T+\varepsilon)\eta=0\ . \tag{4.11b}$$

By multiplying Eq. (4.11b) with σ and then adding it to Eq. (4.11a), we get

$$(E+\sigma F-\varepsilon)(\xi-\sigma\eta)=0\ . \tag{4.12}$$

We must bear in mind that this equation has solutions both for positive and for negative values of ε. Let us first consider the negative eigenvalues for which Eq. (4.12) becomes

$$(E+\sigma F+\varepsilon)[\xi(-\varepsilon)-\sigma\eta(-\varepsilon)]=0,\quad \varepsilon>0\ . \tag{4.13}$$

On the basis of the ket eigenvalue equation (3.11), the operator $(E+\sigma F+\varepsilon)$ cannot have zero eigenvalues, and therefore we must have

$$\xi(-\varepsilon)=\sigma\eta(-\varepsilon),\quad \varepsilon>0\ , \tag{4.14a}$$

or equivalently, using Eq. (4.8),

$$\tilde{\eta}(\varepsilon)=-\sigma\tilde{\xi}(\varepsilon),\quad \varepsilon>0\ . \tag{4.14b}$$

Next we consider Eq. (4.12) for $\varepsilon>0$. We prove that the vector $\xi-\sigma\eta\neq 0$, because if $\xi=\sigma\eta$, and $\eta\neq 0$, then Eq. (4.11b) would give

$$(E^T+F\sigma+\varepsilon)\eta(\varepsilon)=0,\quad \varepsilon>0$$

which is just the transpose of the eigenvalue equation (3.15) for the bra vectors, but with the wrong sign for ε. Since $\eta(\varepsilon)\neq 0$, the above equation cannot be satisfied, and therefore the assumption $\xi(\varepsilon)-\sigma\eta(\varepsilon)=0$ must be wrong for $\varepsilon>0$. Comparing Eqs. (4.12) and (3.11) thus gives the identification

$$X_i^\lambda=\xi_i(\varepsilon_\lambda)-\sum_j{}'\,\sigma_{i+j}\eta_j(\varepsilon_\lambda),\quad \varepsilon_\lambda>0\ . \tag{4.15}$$

Taking into account Eq. (4.14a) and the fact that Eq. (4.11b) is satisfied also for negative ε, we get

$$(E^T+F\sigma-\varepsilon)\eta(-\varepsilon)=0,\quad \varepsilon>0\ . \tag{4.16}$$

This is exactly the eigenvalue equation (3.15) for the bra states, and we can make the identification

$$Y_i^\lambda=\eta_i(-\varepsilon_\lambda)=\tilde{\xi}_i(\varepsilon_\lambda),\quad \varepsilon_\lambda>0\ . \tag{4.17}$$

The results of Eqs. (4.14b), (4.15), and (4.17) are represented pictorially in Fig. 7.

We shall check that the above choices satisfy the normalization condition (3.17),

$$\begin{aligned}\sum_i{}'\,Y_i^\lambda X_i^{\lambda'}&=\sum_i{}'\,\eta_i(-\varepsilon)\left[\xi_i(\varepsilon')-\sum_j{}'\,\sigma_{i+j}\eta_j(\varepsilon')\right]\\&=\sum_i{}'\,[\eta_i(-\varepsilon)\xi_i(\varepsilon')-\xi_i(-\varepsilon)\eta_i(\varepsilon')]\\&=\delta_{\varepsilon,\varepsilon'},\quad \varepsilon=\varepsilon_\lambda \text{ and } \varepsilon'=\varepsilon_{\lambda'}\end{aligned} \tag{4.18}$$

Here use was again made of the result (4.14a) and of the fact that $\varepsilon_\lambda,\varepsilon_{\lambda'}>0$, together with the definition (4.9).

We have shown that there is a one-to-one correspondence between the collective eigenmodes of small oscillations around the equilibrium and the collective bosonic bra and ket excited states. For a fermionic system there exist, of course, also fermionic bra and ket excited states containing odd numbers of extra fermions, which do not show up in the effective Hamiltonian, unless the odd Grassmann amplitudes are also included as briefly discussed in I.

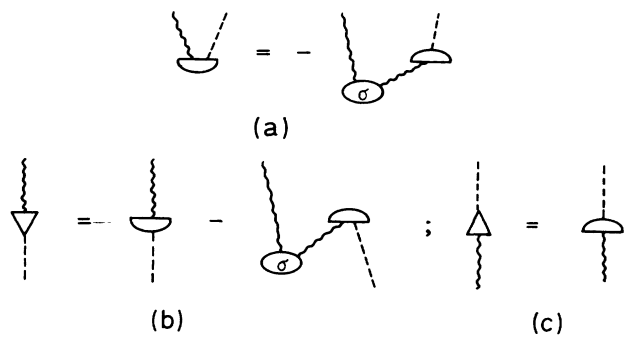

FIG. 7. Diagrammatic representation of the relationships between (a) the left-hand eigenstates $\tilde{\eta}(\varepsilon)$ and $\tilde{\xi}(\varepsilon)$ for $\varepsilon>0$, from Eq. (4.14b); (b) the excited ket-state amplitudes X_i^λ and the right-hand eigenvectors $\xi_i(\varepsilon_\lambda)$ and $\eta_i(\varepsilon_\lambda)$ for $\varepsilon_\lambda>0$, from Eq. (4.15); and (c) the excited bra-state amplitudes Y_i^λ and the left-hand eigenvectors $\tilde{\xi}_i(\varepsilon_\lambda)$ for $\varepsilon_\lambda>0$, from Eq. (4.17).

V. DIAGONALIZATION OF THE EFFECTIVE HAMILTONIAN

When expanded up to the second-order terms in the deviations $\delta\sigma_i(t),\delta\tilde{\sigma}_i(t)$ of the ECCM amplitudes from their respective equilibrium values, the Hamiltonian functional $\bar{H}[\sigma,\tilde{\sigma}]$ describes classical harmonic vibrations of the system around the stationary state. Exactly as in the case of the general harmonic approximation in classical mechanics, e.g., in lattice dynamics, it is possible to diagonalize the vibrational modes by performing a suitable canonical transformation, which introduces the normal coordinates for each individual noninteracting normal mode. In the ECCM functional phase space, discussed in I, this amounts to a coordinate transformation, which is defined locally at the equilibrium point $\{\sigma^0,\tilde{\sigma}^0\}$, but which can also be continued globally to the whole phase space. In terms of the new normal coordinates the Hamiltonian functional recovers a Hermitian form which originally was lost due to the nonunitary nature of the ECCM similarity transformations. In establishing the diagonalizing transformation we shall take advantage of the several orthogonality properties possessed by the previously considered amplitudes $\xi(\varepsilon)$, $\eta(\varepsilon)$, $\tilde{\xi}(\varepsilon)$, and $\tilde{\eta}(\varepsilon)$ on the grounds of the symmetry properties of the dynamical matrix H_D. In the following we shall always restrict ourselves to the positive eigenvalues ε, because for negative ε the amplitudes ξ, η, $\tilde{\xi}$, and $\tilde{\eta}$ simply recover the previous values for the case $\varepsilon>0$ due to Eq. (4.8).

We shall make the strong assumption, true at least in the case of a finite Hilbert space, that the eigenamplitudes ξ, η, $\tilde{\xi}$, and $\tilde{\eta}$ for $\varepsilon>0$ constitute a complete set in the usual sense that an arbitrary block vector indexed by the configuration indices $\{i\}$ can be expanded as

$$\begin{bmatrix}\delta\sigma_i\\ \delta\bar{\sigma}_i\end{bmatrix}=\sum_{\varepsilon}{}^{+}\begin{bmatrix}\xi_i(\varepsilon) & -\bar{\eta}_i(\varepsilon)\\ \eta_i(\varepsilon) & \bar{\xi}_i(\varepsilon)\end{bmatrix}\begin{bmatrix}\psi(\varepsilon)\\ \bar{\psi}(\varepsilon)\end{bmatrix}, \tag{5.1}$$

where the symbol $\sum^{+}$ restricts the summation to positive values of the summation index only. Likewise, here and in the following it is understood that the energy labels ε denote a complete set of quantum indices needed to label a given normal mode, and not just its energy. For a translationally invariant system the proper notation singles out the conserved momentum, and one should denote $\varepsilon\rightarrow\mathbf{q}\varepsilon\nu_1\nu_2\ldots$, where $\nu_1,\nu_2,\ldots$ are any further indices (such as spin, polarization, etc.) needed for a complete specification of the normal mode. In the summations over ε, such as in Eqs. (5.1), (5.3) and (5.4), the conserved momentum $\mathbf{q}$ and other possible conserved indices need not be summed over, since the diagonalization can be made independently in each invariant subspace of vectors $\{\delta\sigma,\delta\bar{\sigma}\}$.

Using the orthonormality relations of Eq. (4.9) the inverse transformation is obviously given by

$$\begin{bmatrix}\psi(\varepsilon)\\ \bar{\psi}(\varepsilon)\end{bmatrix}=\sum_{i}{}'\begin{bmatrix}\bar{\xi}_i(\varepsilon) & \bar{\eta}_i(\varepsilon)\\ -\eta_i(\varepsilon) & \xi_i(\varepsilon)\end{bmatrix}\begin{bmatrix}\delta\sigma_i\\ \delta\bar{\sigma}_i\end{bmatrix}. \tag{5.2}$$

Substituting this expression back into Eq. (5.1) it is possible to express the block identity in the form

$$\begin{bmatrix}I & 0\\ 0 & I\end{bmatrix}=\sum_{\varepsilon}{}^{+}\left\{\begin{bmatrix}\xi(\varepsilon)\\ \eta(\varepsilon)\end{bmatrix}[\bar{\xi}(\varepsilon)^T\ \ \bar{\eta}(\varepsilon)^T]+\begin{bmatrix}-\bar{\eta}(\varepsilon)\\ \bar{\xi}(\varepsilon)\end{bmatrix}[-\eta(\varepsilon)^T\ \ \xi(\varepsilon)^T]\right\}, \tag{5.3}$$

where, again, superscript T denotes the transpose. Spelled out in detail, the following equations are obtained:

$$\delta(i,j)=\sum_{\varepsilon}{}^{+}\{\xi_i(\varepsilon)\bar{\xi}_j(\varepsilon)+\bar{\eta}_i(\varepsilon)\eta_j(\varepsilon)\}, \tag{5.4a}$$

$$0=\sum_{\varepsilon}{}^{+}\{\bar{\eta}_i(\varepsilon)\xi_j(\varepsilon)-\xi_i(\varepsilon)\bar{\eta}_j(\varepsilon)\}, \tag{5.4b}$$

$$0=\sum_{\varepsilon}{}^{+}\{\eta_i(\varepsilon)\bar{\xi}_j(\varepsilon)-\bar{\xi}_i(\varepsilon)\eta_j(\varepsilon)\}. \tag{5.4c}$$

It is possible to express the constituent matrices E, F, and $\bar{F}$ of the dynamical matrix H_D in terms of the eigenvectors. By multiplying H_D from the right with the identity operator (5.3), and using the right-hand eigenvalue equation (4.4) and Eq. (4.8), we find

$$H_D=\sum_{\varepsilon}{}^{+}\left\{\varepsilon\begin{bmatrix}\xi(\varepsilon)\\ \eta(\varepsilon)\end{bmatrix}[\bar{\xi}(\varepsilon)^T\ \ \bar{\eta}(\varepsilon)^T]-\varepsilon\begin{bmatrix}-\bar{\eta}(\varepsilon)\\ \bar{\xi}(\varepsilon)\end{bmatrix}[-\eta(\varepsilon)^T\ \ \xi(\varepsilon)^T]\right\}. \tag{5.5}$$

On comparing with the definition (4.3) of the matrix H_D this reads in detail

$$E=\sum_{\varepsilon}{}^{+}\varepsilon[\xi(\varepsilon)\bar{\xi}(\varepsilon)^T-\bar{\eta}(\varepsilon)\eta(\varepsilon)^T], \tag{5.6a}$$

$$\bar{F}=\sum_{\varepsilon}{}^{+}\varepsilon[\xi(\varepsilon)\bar{\eta}(\varepsilon)^T+\bar{\eta}(\varepsilon)\xi(\varepsilon)^T], \tag{5.6b}$$

$$F=\sum_{\varepsilon}{}^{+}\varepsilon[-\eta(\varepsilon)\bar{\xi}(\varepsilon)^T-\bar{\xi}(\varepsilon)\eta(\varepsilon)^T]. \tag{5.6c}$$

For example, Eq. (5.6b) gives the matrix element

$$\bar{F}_{ij}=\sum_{\varepsilon}{}^{+}\varepsilon[\xi_i(\varepsilon)\bar{\eta}_j(\varepsilon)+\xi_j(\varepsilon)\bar{\eta}_i(\varepsilon)], \tag{5.7}$$

and similarly for the others.

Now it is straightforward to insert Eqs. (5.6) into the second-order Hamiltonian (4.1), and on observing Eq. (5.2) the result will be

$$\bar{H}^{(2)}=E_0+\sum_{\varepsilon}{}^{+}\varepsilon\bar{\psi}(\varepsilon)\psi(\varepsilon) \tag{5.8}$$

for the harmonic Hamiltonian. This equation reveals that the previously introduced amplitudes $\psi,\bar{\psi}$ are indeed the true complex normal-mode amplitudes for the small vibrations. We once more remind the reader that the ε above, as an index, actually stands for a complete set of quantum labels for the normal mode.

As is easily checked, the transformation from the set of variables $\{\delta\sigma,\delta\bar{\sigma}\}$ to the set $\{\psi,\bar{\psi}\}$ is a canonical (or a symplectomorphic) one, and therefore the equations of motion are again obtained in the form

$$i\dot{\psi}(\varepsilon)=\frac{\delta\bar{H}}{\delta\bar{\psi}(\varepsilon)}, \tag{5.9a}$$

$$-i\dot{\bar{\psi}}(\varepsilon)=\frac{\delta\bar{H}}{\delta\psi(\varepsilon)}. \tag{5.9b}$$

In the limit of linear oscillations, the solutions are, using Eq. (5.8),

$$\psi(\varepsilon,t)=e^{-i\varepsilon t}\psi(\varepsilon,0), \tag{5.10a}$$

$$\bar{\psi}(\varepsilon,t)=e^{i\varepsilon t}\bar{\psi}(\varepsilon,0). \tag{5.10b}$$

If the solution is restricted to the physical invariant submanifold corresponding to the Hermitian states in the ECCM phase space, as discussed in I, it is necessary to impose the subsidiary initial condition $\bar{\psi}(\varepsilon,0)=\psi^*(\varepsilon,0)$, where the star denotes complex conjugation. Therefore, at all times the amplitudes $\bar{\psi}$ and ψ remain complex conjugate to each other.

Generalizing now to larger deviations from the equilibrium it is quite possible to continue to use the definition in Eq. (5.1). In the general case it will be necessary to expand the average-value functional to higher powers in $\bar{\psi}$ and ψ. In analogy to the general expression (3.31) of I, we may now write for the average-value functional $\langle A\rangle\equiv\bar{A}$ of an arbitrary operator A,

$$\overline{A}=\overline{A}[\psi,\tilde{\psi}]\equiv\sum_{m=0}^{\infty}\sum_{n=0}^{\infty}\frac{1}{m!n!}\sum_{\{\varepsilon'\}}^{+}\sum_{\{\varepsilon\}}^{+}\langle\varepsilon'_1\cdots\varepsilon'_m\mid A\mid\varepsilon_1\cdots\varepsilon_n\rangle\tilde{\psi}(\varepsilon'_1)\cdots\tilde{\psi}(\varepsilon'_m)\psi(\varepsilon_n)\cdots\psi(\varepsilon_1)\ . \tag{5.11}$$

Here the matrix elements $\langle\cdots\mid A\mid\cdots\rangle$ are functionals of the equilibrium amplitudes $\sigma^0,\tilde{\sigma}^0$ and of the configuration-space matrix elements $\langle i_1\cdots i_m\mid A\mid j_1\cdots j_n\rangle$ and it is to be understood that for $m=n=0$, $\langle\mid A\mid\rangle=\overline{A}_0$, the equilibrium value. The Hamiltonian, for example, will be

$$\begin{aligned}\overline{H}=&E_0+\sum_{\varepsilon}^{+}\varepsilon\tilde{\psi}(\varepsilon)\psi(\varepsilon)\\&+\sum_{\varepsilon_1\varepsilon_2\varepsilon_3}^{+}\left[\tfrac{1}{6}\langle\varepsilon_1\varepsilon_2\varepsilon_3\mid H\mid\rangle\tilde{\psi}(\varepsilon_1)\tilde{\psi}(\varepsilon_2)\tilde{\psi}(\varepsilon_3)+\tfrac{1}{2}\langle\varepsilon_1\varepsilon_2\mid H\mid\varepsilon_3\rangle\tilde{\psi}(\varepsilon_1)\tilde{\psi}(\varepsilon_2)\psi(\varepsilon_3)+\tfrac{1}{2}\langle\varepsilon_1\mid H\mid\varepsilon_2\varepsilon_3\rangle\tilde{\psi}(\varepsilon_1)\psi(\varepsilon_3)\psi(\varepsilon_2)\right.\\&\left.+\tfrac{1}{6}\langle\mid H\mid\varepsilon_1\varepsilon_2\varepsilon_3\rangle\psi(\varepsilon_3)\psi(\varepsilon_2)\psi(\varepsilon_1)\right]+O(\mid\psi\mid^4)\ .\end{aligned} \tag{5.12}$$

The matrix elements in Eq. (5.11) may be more precisely given in terms of the equilibrium values of the functional derivatives of $\langle A\rangle$ as

$$\langle\varepsilon'_1\cdots\varepsilon'_m\mid A\mid\varepsilon_1\cdots\varepsilon_n\rangle=\frac{\delta^{m+n}}{\delta\tilde{\psi}(\varepsilon'_1)\cdots\delta\tilde{\psi}(\varepsilon'_m)\delta\psi(\varepsilon_1)\cdots\delta\psi(\varepsilon_n)}\langle A\rangle\mid_{\psi=\tilde{\psi}=0}\ . \tag{5.13}$$

These may in turn be expressed as functional derivatives with respect to the original amplitudes $\{\sigma,\tilde{\sigma}\}$, using the relations

$$\frac{\delta}{\delta\tilde{\psi}(\varepsilon)}=\sum_i{}'\left[\tilde{\xi}_i(\varepsilon)\frac{\delta}{\delta\tilde{\sigma}_i}-\tilde{\eta}_i(\varepsilon)\frac{\delta}{\delta\sigma_i}\right]\ , \tag{5.14a}$$

$$\frac{\delta}{\delta\psi(\varepsilon)}=\sum_i{}'\left[\eta_i(\varepsilon)\frac{\delta}{\delta\tilde{\sigma}_i}+\xi_i(\varepsilon)\frac{\delta}{\delta\sigma_i}\right]\ . \tag{5.14b}$$

It may be instructive to give a diagrammatical representation for typical normal-mode matrix elements of an operator, such as appear in Eq. (5.11). These are shown in Fig. 8, using the diagrammatic elements previously introduced in Sec. IV.

The equation of motion for an average value of an operator can still be given with the aid of a generalized Poisson-bracket expression in analogy to the similar result in I,

$$\frac{d}{dt}\overline{A}=\overline{\frac{\partial A}{\partial t}}+\{\overline{A},\overline{H}\}\ , \tag{5.15}$$

where one now defines

$$i\{\overline{A},\overline{H}\}\equiv\sum_{\varepsilon}^{+}\left[\frac{\delta\overline{A}}{\delta\psi(\varepsilon)}\frac{\delta\overline{H}}{\delta\tilde{\psi}(\varepsilon)}-\frac{\delta\overline{H}}{\delta\psi(\varepsilon)}\frac{\delta\overline{A}}{\delta\tilde{\psi}(\varepsilon)}\right]\ . \tag{5.16}$$

Formally, Eq. (5.12) together with the equations of motion form a quasilocal classical field theory with nonlinear couplings between the normal modes. It bears similarity to an anharmonic dynamical lattice system as well as to the well-known Ginzburg-Landau-type effective field theories, where the function ψ is an order parameter, although obvious factual differences naturally prevail. It is conceivable that in a suitable infrared or long-wavelength limit the present quasilocal field theory may look completely local.

We note also that—even though the system obeys Hamiltonian dynamics—the formalism has its own built-in mechanism for possible dissipation of the vibrations, namely, through the higher-order nonlinear coupling terms. These will lead to such possible phenomena as, for example, frequency splittings and redistribution of the energy among the normal modes. According to the simplest possible scenario, which assumes ergodicity, we may find that, if the initial energy of a sufficiently large system exceeds the ground-state energy by an (in the thermodynamic sense) extensive quantity, the final outcome after a long time will be a temporally fluctuating system in which the total energy is distributed among the various normal modes in the average according to an appropriate statistical distribution. In case of a finite, nonextensive excess energy, the nonlinear interactions can shift energy

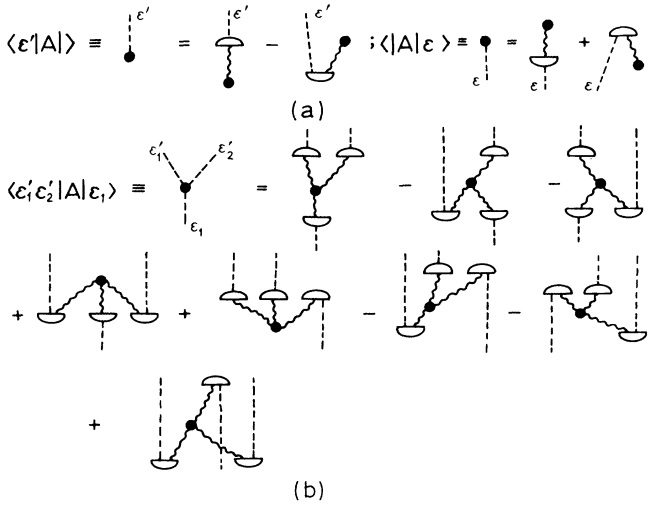

FIG. 8. Diagrammatic representation of the normal-mode matrix elements (5.13) of an operator, where the solid vertex dots with wavy tails represent equilibrium values of the functional derivatives of $\langle A\rangle$ with respect to $\{\sigma,\tilde{\sigma}\}$. The simplest elements $\langle\mid A\mid\varepsilon\rangle$ and $\langle\varepsilon'\mid A\mid\rangle$ shown in (a) illustrate the general rules for constructing the more general elements, a typical example of which is shown in (b).

into the low-energy infrared modes, leaving the system ultimately in its zero-temperature ground state. We shall not, however, expand the present discussion further into the direction of statistical physics, which in principle would require a careful study of the trajectories and of the flow of the representative phase-space points in the ECCM phase space.

In making the coordinate transformation in the ECCM phase space into the locally normal coordinates around the equilibrium point $\{\sigma_i^0,\tilde{\sigma}_i^0\}$ it was nowhere assumed that the equilibrium state should have the same maximal symmetry as the original Hamiltonian. The above general equations are therefore valid also for small (mesonlike) oscillations around an equilibrium state where some topological objects may be present, such as vortices, kinks, solitons, or surfaces, depending on the system in question.

VI. SUMMARY AND DISCUSSION

We showed in I how, in a very definite sense, an arbitrary quantum theory with a Schrödinger dynamics is made classical by applying the ECCM to it. Thus, the quantum theory is exactly mapped into a classical field theory which comprises a set of (configuration-space indexed) many-body, quasilocal, classical (i.e., c-number) fields $\{\sigma_i,\tilde{\sigma}_i\}$, which interact via nonlocal classical interactions. We have now extended the ECCM parametrization of the ground state (specified completely in terms of the amplitudes $\{\sigma_i,\tilde{\sigma}_i\}$) given in I, to describe excited states also.

In particular, we have shown in Sec. III how the new ECCM amplitudes that we introduce to parametrize the excited states are formulated as the solutions of a set of linear eigenvalue equations in the ECCM configuration space. The coefficients in these equations are completely specified by the amplitudes $\{\sigma_i,\tilde{\sigma}_i\}$ defined with respect to the ground state, and the eigenvalues give the excitation energies directly rather than as the absolute energy for the excited state (which would then need to have subtracted from it the ground-state energy determined previously).

Since the formalism discussed in I gave a general dynamic description of a quantum many-body system, we exploited this aspect in Sec. IV to consider small oscillations of the system around its stable equilibrium ground state. In particular, we proved that there is a one-to-one equivalence between these small-oscillation (linear-response) collective eigenmodes and the previous collective excited states discussed in Sec. III. Furthermore, we showed how the effective Hamiltonian approach to small oscillations around the stationary point also leads to an exact generalization of the well-known RPA. This generalized RPA scheme itself reinforces our earlier interpretation of the amplitudes $\{\sigma_i,\tilde{\sigma}_i\}$ as a set of generalized, classical mean fields, which completely and exactly characterize the original quantum-mechanical many-body system in its ground state.

The normal RPA has been very successfully applied in the past to the study of elementary excitations in such many-body systems as the electron gas, finite atomic nuclei, and nuclear matter. In perturbation-theoretic terms, the diagrams included in RPA are also used to calculate corrections to the ground-state energy and to investigate the coupling of the excited states to the collective modes and the particle-hole excitations of the system. However, when the basic microscopic interparticle forces are strong, the input to the normal RPA has usually been not the bare interaction, but some phenomenological particle-hole interaction, such as a local approximation to some effective Brueckner G matrix or a Skyrme interaction. Our own formulation, on the other hand, in principle circumvents this problem and remains fully microscopic. In this respect, it may perhaps most closely be compared with the so-called correlated-RPA (CRPA) method,[15] which is formulated within the general framework of the method of correlated basis functions (CBF).[16–19] It has been shown[15] how the CBF-CRPA method may also be derived from the dynamic variational principle for the action, as used in I. Instead of being applied to the ECCM-parametrized states as in I, in the CBF-CRPA method it is applied to a class of correlated states which are especially designed to build in strong short-range correlations from the outset. A typical example of such states are the well-known Jastrow states. For future applications of our own generalized RPA it may be interesting to attempt a comparison of our own effective Hamiltonian with the comparable effective interaction that arises in the CBF-CRPA method. We do not attempt such a discussion here however.

Finally, in Sec. V, we carried the ECCM approach to the collective eigenmodes of linear response to its logical conclusion, by explicitly diagonalizing the corresponding effective Hamiltonian curtailed at second-order terms in the deviations, $\delta\sigma_i(t)$ and $\delta\tilde{\sigma}_i(t)$, of the ECCM amplitudes from their stationary ground-state values. In this way the system is reduced to a collection of noninteracting classical harmonic oscillators. We also went beyond this harmonic approximation and showed how the complete (untruncated) Hamiltonian functional could be reexpressed in terms of the normal modes of the quadratic effective Hamiltonian. In this way, the original quantal Hamiltonian formalism is mapped into a classical field theory with nonlinear (anharmonic) couplings of arbitrarily high order between the normal modes in the ECCM configuration space. A consequence of this reformulation in terms of normal configuration-space coordinates, is that the Hamiltonian functional, which previously was not manifestly Hermitian due to the nonunitary nature of the underlying ECCM similarity transformations, is now rendered explicitly Hermitian.

In this final form, the present theory may be compared with the Ginzburg-Landau phenomenology. This expresses the total energy (or free energy for nonzero temperatures) as a strictly local functional (restricted to fourth-order terms) of the one-body (local) "order parameters" $\langle a^\dagger(\mathbf{x})\rangle=\tilde{\sigma}_1(\mathbf{x})$ and $\langle a(\mathbf{x})\rangle=\sigma_1(\mathbf{x})$, which are the ground-state expectation values for the single-particle creation and destruction operators in coordinate space. Our own ECCM approach clearly incorporates the complete set of amplitudes $\{\sigma_i,\tilde{\sigma}_i\}$, which may from this viewpoint be regarded as order parameters of arbitrary complexity. We remind ourselves, however, that whereas

the Ginzburg-Landau approach is only intended to be applicable in a region close to the associated phase transition where the order parameters are small, our own ECCM formalism is an exact microscopic description of an arbitrary pure quantum state, and hence of a system at zero temperature.

Despite its formulation here and in I in terms of a rather general nonlinear algebraic structure, and despite being based (in I) on a dynamic variational principle, the ECCM has its origins in, and continues to have strong links with, perturbation theory. With respect to a given model state, we have seen how it represents, both exactly and at various truncation levels, a precise summation of certain classes of linked perturbation-theory diagrams. These can be represented as well-defined tree-diagram structures with certain maximal generalized time-ordering properties.[1,2] A consequence is that every low-order perturbation diagram is always kept together with an associated infinite class of diagrams corresponding to arbitrarily high-order perturbation theory, even at very low levels of truncation in the ECCM configuration space. It is this feature which ultimately enables the method to transcend its origins, and to describe such phenomena as phase transitions or topological excitations, which cannot be treated by finite-order perturbation theory.

It is perhaps also worth pointing out that the ECCM perturbation-theory diagrams are always connected with a well-defined particular state of the system. This is not always the case with other diagrammatic methods. As developed in I, this state is the ground state in the first place, where the basic amplitudes $\{\sigma_i,\tilde{\sigma}_i\}$ (or $\{S_i,S_i''\}$) are used to parametrize the ground state; and we have seen in the present paper how the formalism may be extended to excited states.

Although we have not explicitly constructed them here, it should be clear that the present formalism may rather readily be extended to construct the chronological Green functions, which are themselves intimately connected with the oscillations of the system about its stable equilibrium state. In this regard it might be interesting to attempt a more detailed comparison of the ECCM truncation systematics with other methods employing Green functions and approximations based on them. An obvious candidate for such a comparison is the parquet diagram method,[20] which has been particularly successful in applications to many-boson systems.

By imbedding the theory of linear response within the normal CCM, one of us has previously shown[12] how each of the usual sum rules for the energy-weighted moments of the dynamic structure function can be exactly decomposed into an infinite hierarchy of sub-sum-rules which relate the ground- and excited-state CCM correlation amplitudes to one another. Similar discussions concerning sum rules and conservation laws may also be attempted within the ECCM. In a future paper we intend, for example, to apply the ECCM to the case of a condensed Bose fluid. We shall show how the ECCM may be applied to a general nonuniform and time-varying system. In particular we shall demonstrate how the method may be used to provide a completely gauge-invariant description of such systems, and consequently also a complete hydrodynamical description in the zero-temperature limit. We shall show how the hydrodynamical balance equations for such local observables as the number density, momentum density, and energy density can be exactly formulated, not only for the exact (untruncated) formalism, but also for various practical truncation schemes in the ECCM configuration space. In this way we are able to offer a complete hydrodynamical description of the zero-temperature Bose fluid, which in principle includes a proper account of such phenomena as topological deformations and nonequilibrium processes.

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