Extended coupled-cluster method. III. Zero-temperature hydrodynamics of a condensed Bose fluid

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The extended coupled-cluster method (ECCM) of quantum many-body theory, which has been studied and developed in earlier papers in this series, is now applied to condensed Bose systems. The formalism is seen to provide a concise and convenient description of quite general nonstatic states of such systems with arbitrary spatial inhomogeneity. The entire ECCM description is based on the equations of motion for the set of linked-cluster amplitudes which, we have shown, completely characterize an arbitrary quantum system with a Schrödinger dynamics. Since all such amplitudes obey the cluster property, and hence may be regarded as a set of quasilocal, many-body, classical order parameters, the formalism is in principle perfectly capable of describing phase transitions and states of topological excitation or deformation and broken symmetry. At the lowest (mean-field) level of truncation, the formalism degenerates to the well-known Gross-Pitaevskii description of the condensate wave function or one-body order parameter. The treatment is developed in a fully gauge-invariant fashion, and is thereby shown to provide a complete hydrodynamical description, valid in the zero-temperature limit. In particular, by studying the off-diagonal one- and two-body density matrices in terms of the basic ECCM amplitudes, we derive balance (or local conservation) equations for such local observables as the number density, momentum density, and energy density. These are shown to be obeyed not only by the exact untruncated formalism but also by most practical truncation schemes in the ECCM configuration space.

I. INTRODUCTION

In two previous papers,[1,2] henceforth referred to as I and II, respectively, we have discussed the extended coupled-cluster method (ECCM) of quantum many-body theory in considerable detail. We showed that the formalism could be formulated in such a fashion as to be applicable to any many-body system for which a Schrödinger dynamics is defined. Furthermore, we demonstrated how the ECCM provides an extremely convenient parametrization of the entire Hilbert space appropriate to any such system.

The discussion in I largely focused on general properties of the formalism, and was centered on the calculation of ground-state expectation values of arbitrary operators. We showed how such average values could be expressed entirely in terms of the basic linked-cluster amplitudes $\{\sigma_n,\tilde{\sigma}_n\}$ which serve as a complete parametrization of the many-body system within the ECCM. Although the presentation in I proceeded from the starting point of a dynamic variational principle, and was couched in the language of a formally exact set of nonlinear coupled equations of motion for the basic amplitudes $\{\sigma_n,\tilde{\sigma}_n\}$, the ECCM is nevertheless still deeply rooted in perturbation theory, in a fashion similar to the more well-known normal coupled-cluster method [or exp(S) method] of Coester and Kümmel,[3-6] from which it derives.[7]

It has been shown[7] that the ECCM may be viewed as a particular complete summation scheme for the entire class of Goldstone diagrams of time-independent perturbation theory, defined with respect to some particular model state. One very useful feature[1,7] is that the ECCM naturally groups these diagrams as generalized time-ordered (GTO) tree diagrams, where the GTO property runs both forwards and backwards in time. Furthermore, at each level of approximation the average value $\langle A \rangle$ of an arbitrary operator A is obtainable within the ECCM from precisely the same set of Goldstone diagrams as the energy, by replacing each Hamiltonian interaction in turn by the operator A.

The capability of interpreting the ECCM in terms of

Goldstone perturbation theory can be very useful for comparisons with other methods, and for purposes of interpretation of the physical content of various approximations. However, we stress that such comparisons or interpretations are never actually necessary. We were at pains in our earlier papers to stress that the ECCM now undoubtedly so far transcends its perturbation-theoretic origins as to be (at least potentially) capable of describing such intrinsically nonperturbative phenomena as spontaneous symmetry breaking, phase transitions, topological excitations and deformations, and nonequilibrium processes. In perturbation-theory terms, this is achieved by the natural groupings of diagrams which the method imposes. Thus, every low-order perturbation-theoretic diagram is always associated with an infinite class of higher-order diagrams in such a way that the basic amplitudes always obey the cluster property—namely, that they become zero in the limit that any subset of the particles described by the amplitude becomes far removed from the remainder. Such a strict observance of the cluster property is vital for a proper description of many nonperturbative phenomena. For example, it is clearly necessary for a proper imposition of the topological boundary conditions which characterize such objects as a vortex line in liquid helium, or quite general soliton excitations in condensed matter systems.

We showed in particular in I how the ECCM served to map an arbitrary quantum many-body theory onto a classical Hamiltonian mechanics of the classical, many-body, quasilocal fields $\{\sigma_n,\tilde{\sigma}_n\}$. Further, we showed how the ECCM could also be interpreted as an exact generalized mean-field theory of the original quantal system. Indeed, at its lowest level of truncation (which keeps only the one-body amplitudes σ_1 and $\tilde{\sigma}_1$), the ECCM degenerates into the usual mean-field theory or semiclassical approximation.

The ground-state formalism of I was extended in II to deal with excited states, and in particular the role of the basic amplitudes $\{\sigma_n,\tilde{\sigma}_n\}$ as a set of generalized collective coordinates for the system was thereby further clarified. We showed also how the excitation spectrum could be obtained by considering small oscillations around the equilibrium configuration. The effective Hamiltonian that describes this situation was shown to have the structure of an exact generalization of the well-known random-phase approximation of Bohm and Pines.[8] We diagonalized this effective Hamiltonian and thereby were able to express arbitrary behavior of the system in terms of these small oscillation normal coordinates. As an example, we showed how the energy of the system, calculated as the exact average-value functional of the Hamiltonian, has a structure quite comparable to that in the phenomenological Ginzburg-Landau theory.

In the present paper we intend to apply the general formalism of the earlier papers to the special case of a condensed Bose system. Formally, such systems are among the simplest and cleanest quantal many-body systems available for study; although one knows that in practice such systems as liquid ^{4}He are among the most difficult to describe quantitatively for even such basic quantities as the ground-state energy as a function of density. The reason for this ultimately lies in the difficulty of designing suitable truncation or approximation schemes. In this respect one would ideally like the same approximation to be applicable to all quantities of interest, and the aforementioned property of the ECCM that the expectation value $\langle A \rangle$ for an arbitrary operator A is completely compatible with the energy expectation value now assumes particular significance.

Also of historical importance in developing new approximation schemes has been the preservation or otherwise of various exact conservation laws and sum rules. One of the main motivations of the present paper has similarly stemmed from such considerations. Our intention is to show how the ECCM may be applied to a general, spatially nonuniform and nonstatic system. In particular, the formalism is developed to provide a completely gauge-invariant description of such systems and, thence, also a complete hydrodynamical description, applicable in the zero-temperature limit. Our aim here is less to design specific approximations for particular systems, than to investigate how the various hydrodynamical balance equations or local conservation laws can be formulated both in the exact formalism as well as in quite general classes of approximation schemes.

The plan of the remainder of the paper is as follows. The basic ECCM formalism is first reviewed in Sec. II insofar as it is necessary for present purposes. We describe in Sec. III how the standard Bogoliubov prescription[9–12] for the macroscopic occupation of the condensate is imbedded within the present ECCM formalism by explicitly breaking the underlying gauge symmetry which arises from particle-number conservation. This is achieved by choosing the particle vacuum as the model (uncorrelated) state, so that the subsequent ECCM wave functions describe states of indefinite particle number. The number conservation must, however, be taken properly into account when coupling the system to external scalar and vector gauge fields $\phi(\mathbf{r},t)$ and $\mathbf{A}(\mathbf{r},t)$. We show that these fields can be interpreted as providing differential or local Galilean transformations which vary with position in the system. A proper hydrodynamical description must then be able to distinguish in a gauge-invariant fashion between, for example, the local hydrodynamical kinetic energy density of translation from the intrinsic kinetic energy density in the local rest frame.

In Sec. IV we derive the equations of motion for the basic linked-cluster amplitudes $\{\sigma_n,\tilde{\sigma}_n\}$, and from these also the equation of motion for the general off-diagonal elements $\bar{\rho}(\mathbf{r},\mathbf{r}')$ of the one-body density operator. We describe how the set of coupled equations for the basic amplitudes $\{\sigma_n,\tilde{\sigma}_n\}$ may be regarded as an exact generalization of the approximate Gross-Pitaevskii[13–15] nonlinear equations appropriate to weakly interacting condensed Bose systems. The transformation properties of the one-body density matrix under gauge transformations are then investigated in Sec. V, and the equation of motion for $\bar{\rho}(\mathbf{r},\mathbf{r}')$ is thereby expanded in gauge-invariant quantities up to second-order terms in the difference $\boldsymbol{\xi}=\mathbf{r}-\mathbf{r}'$ as this quantity approaches zero.

The physical content of these equations is then analyzed in Sec. VI. In particular, we show how the local

conservation equations for such local observables as the number density, momentum density, and energy density can thereby be formulated and shown to be satisfied not only for the untruncated (and hence exact) formalism, but also for various practical truncation schemes in the ECCM configuration space. In this way we show that the ECCM provides a complete hydrodynamical description of the zero-temperature condensed Bose fluid. The formalism is powerful enough to be able to describe such phenomena as topological excitations and nonequilibrium processes. Finally, in Sec. VII we present a summary and discussion of our results.

II. THE BASIC ECCM FORMALISM

As we have seen in I and II, and as summarized again below, one of the fundamental underlying themes of the ECCM is the double similarity transformation generated by the basic operators which are used in the formalism to parametrize the many-body states. The basic similarity transformation is not unitary, and hence the ECCM is not a manifestly Hermitian theory. Of course, in an exact formulation of the ECCM in which no approximations were made to implement it, all expectation values of Hermitian operators belonging to physically observable quantities would remain real. We showed in II how the method may be viewed as a biorthogonal formulation of the quantum many-body problem. In any case, it is best from the outset not to restrict ourselves to many-body Hamiltonians or their relevant subsequent transforms that are necessarily Hermitian.

Hence, with complete generality we may denote the equilibrium ground-state bra and ket states of the exact many-body Hamiltonian H as $\langle \Psi_0' |$ and $| \Psi_0 \rangle$, respectively, where

$$H | \Psi_0 \rangle = E_0 | \Psi_0 \rangle, \quad \langle \Psi_0' | H = E_0 \langle \Psi_0' | \ , \tag{2.1}$$

corresponding to the ground-state energy E_0. Similarly, if the system is not in equilibrium (or if the Hamiltonian itself is time dependent), we must use the time-dependent Schrödinger equations instead of Eq. (2.1). These may themselves be formulated as a dynamic variational principle based on an actionlike functional,

$$\mathcal{A} = \mathcal{A}[\Psi, \Psi'] \equiv \int dt \langle \Psi'(t) | (i\partial/\partial t - H) | \Psi(t) \rangle \ . \tag{2.2}$$

Stationarity of $\mathcal{A}$ with respect to small variations in the independent states $| \Psi(t) \rangle$ and $\langle \Psi'(t) |$, subject only to the vanishing of $| \delta\Psi(t) \rangle$ and $\langle \delta\Psi'(t) |$ at the implied end points of the time integral in Eq. (2.2) (usually $t \to \pm\infty$), then gives the correct Schrödinger equations of motion,

$$\begin{aligned} &\delta\mathcal{A}/\delta\Psi' = 0 \Longrightarrow i(\partial/\partial t) | \Psi(t) \rangle = H | \Psi(t) \rangle \ , \\ &\delta\mathcal{A}/\delta\Psi = 0 \Longrightarrow -i(\partial/\partial t) \langle \Psi'(t) | = \langle \Psi'(t) | H \ . \end{aligned} \tag{2.3}$$

The ECCM may now be formulated as a particular parametrization of the states $| \Psi(t) \rangle$ and $\langle \Psi'(t) |$ in terms of a set of fully linked configuration-space amplitudes, each of which obeys the very important cluster property that it tends to zero as any subset of the particles, described by the particular configuration, becomes far removed from the remainder. As is typical of a large class of quantum-mechanical calculations, the ECCM employs a construction of an arbitrary state in the full Hilbert space $\mathcal{H}$, which is based on some suitable initial or model state $| \Phi \rangle$. This is often, but by no means necessarily, chosen to be some suitable state in which the system would otherwise be when (some part of) the interactions are turned off. Within the ECCM, the only assumption placed on $| \Phi \rangle$ is that it is a cyclic vector. We assume furthermore that the algebra of all operators in $\mathcal{H}$ is spanned by the two Abelian subalgebras of the many-body configuration-space creation and destruction operators, defined with respect to the given state $| \Phi \rangle$. The basic assumption is therefore 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 many-body configuration-space creation-operator subalgebra; and similarly for the bra states with respect to $\langle \Phi |$ and the destruction-operator subalgebra.

In the above context, we discussed in detail in I the very considerable merits of the ECCM parametrization of the states,

$$| \Psi(t) \rangle = e^{\phi(t)} e^{S(t)} | \Phi \rangle = e^{\phi(t)} e^{S(t)} e^{-S''(t)} | \Phi \rangle \ , \tag{2.4a}$$

$$\langle \Psi'(t) | = e^{-\phi(t)} \langle \Phi | e^{S''(t)} e^{-S(t)} \ . \tag{2.4b}$$

The important content of Eqs. (2.4) is that the operators $S(t)$ and $S''(t)$ are built, respectively, only of creation and destruction operators (defined, as above, with respect to the cyclic vector $| \Phi \rangle$), namely,

$$S''(t) | \Phi \rangle = 0 = \langle \Phi | S(t) \ , \tag{2.5}$$

whence follows the second equality in Eq. (2.4a), and with amplitudes that in both cases are linked-cluster quantities. The factor $\phi(t)$ in Eqs. (2.4) is some, largely irrelevant, appropriate c-number scale factor. It follows immediately from Eqs. (2.4) that the normalization condition,

$$\langle \Psi'(t) | \Psi(t) \rangle = 1 \ , \tag{2.6}$$

is preserved for all times. It follows that the average-value or expectation-value functional of an arbitrary operator A

$$\langle A \rangle \equiv \overline{A}(t) \equiv \langle \Psi'(t) | A | \Psi(t) \rangle \ , \tag{2.7}$$

may also be written as a model-state expectation value of the doubly similarity-transformed operator $\hat{A}(t)$ already alluded to above, and now defined as

$$\begin{aligned} &\langle A \rangle = \langle \Phi | \hat{A}(t) | \Phi \rangle \ , \\ &\hat{A}(t) \equiv e^{S''(t)} e^{-S(t)} A e^{S(t)} e^{-S''(t)} \ . \end{aligned} \tag{2.8}$$

In the remainder of the present work we shall henceforth choose the cyclic state $| \Phi \rangle$ to be the bare vacuum state. Accordingly, we shall be working in a number-nonconserving formulation, as introduced by Bogoliubov.[9] The many-body configuration space will be parametrized by real-space coordinate indices. We assume for ease that the bosons are spinless, but it would be a trivial matter to add spin indices if required. The basic single-boson creation and destruction operators $a_x^\dagger$

and a_x, which respectively, create and destroy a particle at the three-space point $x \equiv (x^1, x^2, x^3)$, obey the usual canonical commutation relations,

$$[a_x, a_y^\dagger] = \delta^{(3)}(x-y) \equiv \delta(x-y) \ . \tag{2.9}$$

For notational simplicity, we denote three vectors in coordinate space as $r, r', x_1, x_2, \ldots$ and corresponding volume elements as $dr, dr', dx_1, dx_2, \ldots$. In the many-body Hilbert space $\mathcal{H}$, with fixed particle number N, the identity operator I then has the following resolution in this coordinate-space representation:

$$I = \sum_{n=0}^{\infty} \frac{1}{n!} \int dx_1 \cdots \int dx_n a_{x_1}^\dagger \cdots a_{x_n}^\dagger \mid \Phi \rangle \times \langle \Phi \mid a_{x_n} \cdots a_{x_1} \ , \tag{2.10}$$

in which the $n=0$ term is simply a shorthand notation for the term $\mid \Phi \rangle \langle \Phi \mid$. Similarly, the basic ECCM operators $S(t)$ and $S''(t)$ have the representations

$$S(t) \equiv \sum_{n=1}^{\infty} \frac{1}{n!} \int dx_1 \cdots \int dx_n S_n(x_1, \ldots, x_n; t) \times a_{x_1}^\dagger \cdots a_{x_n}^\dagger \ , \tag{2.11}$$

$$S''(t) \equiv \sum_{n=1}^{\infty} \frac{1}{n!} \int dx_1 \cdots \int dx_n S_n''(x_1, \ldots, x_n; t) \times a_{x_n} \cdots a_{x_1} \ ,$$

in which the linked-cluster amplitudes $S_n(x_1, \ldots, x_n; t)$ and $S_n''(x_1, \ldots, x_n; t)$ may, with no loss of generality, be assumed symmetric under the interchange of any two coordinate-space arguments, and which hence have the explicit form

$$S_n(x_1, \ldots, x_n; t) = \langle \Phi \mid a_{x_n} \cdots a_{x_1} S(t) \mid \Phi \rangle \ ,$$
$$S_n''(x_1, \ldots, x_n; t) = \langle \Phi \mid S''(t) a_{x_1}^\dagger \cdots a_{x_n}^\dagger \mid \Phi \rangle \ . \tag{2.12}$$

It has also been pointed out in I that it is more convenient to use an equivalent pair of operators $\Sigma(t)$ and $\tilde{\Sigma}(t) \equiv S''(t)$, rather than the above operators $S(t)$ and $S''(t)$, and in terms of which most of the resulting equations have a more symmetric form. They are defined as

$$\Sigma(t) \equiv \sum_{n=1}^{\infty} \frac{1}{n!} \int dx_1 \cdots \int dx_n \sigma_n(x_1, \ldots, x_n; t) \times a_{x_1}^\dagger \cdots a_{x_n}^\dagger \ , \tag{2.13}$$

$$\tilde{\Sigma}(t) \equiv \sum_{n=1}^{\infty} \frac{1}{n!} \int dx_1 \cdots \int dx_n \tilde{\sigma}_n(x_1, \ldots, x_n; t) \times a_{x_n} \cdots a_{x_1} \ ,$$

in terms of matrix elements given as

$$\sigma_n(x_1, \ldots, x_n; t) \equiv \langle \Phi \mid a_{x_n} \cdots a_{x_1} e^{S''(t)} S(t) \mid \Phi \rangle \ ,$$
$$\tilde{\sigma}_n(x_1, \ldots, x_n; t) \equiv \langle \Phi \mid S''(t) a_{x_1}^\dagger \cdots a_{x_n}^\dagger \mid \Phi \rangle = S_n''(x_1, \ldots, x_n; t) \ . \tag{2.14}$$

The matrix elements $\sigma_n(x_1, \ldots, x_n; t)$ and $\tilde{\sigma}_n(x_1, \ldots, x_n; t)$ are again completely symmetric with respect to arbitrary permutations of the coordinate-space vectors $x_1, \ldots, x_n$. A comparison of Eqs. (2.12)–(2.14), together with the resolution (2.10) of the identity, shows that

$$\Sigma(t) \mid \Phi \rangle = [e^{S''(t)} S(t) - \langle \Phi \mid e^{S''(t)} S(t) \mid \Phi \rangle] \mid \Phi \rangle \ , \tag{2.15}$$

which in turn, together with use of Eq. (2.5), gives the inverse transformation as

$$[S(t) - \langle \Phi \mid e^{S''(t)} S(t) \mid \Phi \rangle] \mid \Phi \rangle = e^{-\tilde{\Sigma}(t)} \Sigma(t) \mid \Phi \rangle \ , \tag{2.16a}$$

or, by making use of Eq. (2.12), equivalently as

$$S_n(x_1, \ldots, x_n; t) = \langle \Phi \mid a_{x_n} \cdots a_{x_1} e^{-\tilde{\Sigma}(t)} \Sigma(t) \mid \Phi \rangle \ . \tag{2.16b}$$

The entire ECCM formalism may now be fully formulated in terms of the set of amplitudes $\{\sigma_n(x_1, \ldots, x_n; t), \tilde{\sigma}_n(x_1, \ldots, x_n; t)\}$, which play the role of a complete set of (c-number) dynamic variables. For example, an arbitrary average-value functional as defined in Eqs. (2.7) and (2.8) is now specified as $\langle A \rangle \equiv \bar{A} = \bar{A}[\sigma_n, \tilde{\sigma}_n]$. It is also straightforward to show that the action functional of Eq. (2.2) can be expressed as

$$\mathcal{A} = \int dt [i \langle \Phi \mid \tilde{\Sigma}(t) \dot{\Sigma}(t) \mid \Phi \rangle - \bar{H}] \tag{2.17a}$$

$$= \int dt [-i \langle \Phi \mid \dot{\tilde{\Sigma}}(t) \Sigma(t) \mid \Phi \rangle - \bar{H}] \ , \tag{2.17b}$$

where we have employed an integration by parts. In terms of the parametrizations of Eqs. (2.13), the action becomes

$$\mathcal{A} = i \int dt \sum_{n=1}^{\infty} \frac{1}{n!} \int dx_1 \cdots \int dx_n \tilde{\sigma}_n(x_1, \ldots, x_n; t) \dot{\sigma}_n(x_1, \ldots, x_n; t) - \int dt \, \bar{H}[\sigma_n, \tilde{\sigma}_n] \tag{2.18a}$$

$$= -i \int dt \sum_{n=1}^{\infty} \frac{1}{n!} \int dx_1 \cdots \int dx_n \dot{\tilde{\sigma}}_n(x_1, \ldots, x_n; t) \sigma_n(x_1, \ldots, x_n; t) - \int dt \, \bar{H}[\sigma_n, \tilde{\sigma}_n] \ . \tag{2.18b}$$

The requirement that $\mathcal{A}$ be stationary with respect to variations in each of the amplitudes $\bar{\sigma}_n(x_1,\ldots,x_n;t)$ and $\sigma_n(x_1,\ldots,x_n;t)$ then leads, respectively, to the equations of motion

$$i\dot{\sigma}_n(x_1,\ldots,x_n;t)=\delta\bar{H}/\delta\bar{\sigma}_n(x_1,\ldots,x_n;t)\ , \tag{2.19a}$$

$$-i\dot{\bar{\sigma}}_n(x_1,\ldots,x_n;t)=\delta\bar{H}/\delta\sigma_n(x_1,\ldots,x_n;t)\ . \tag{2.19b}$$

At the stationary point, the equilibrium values of each of the amplitudes σ_n and $\bar{\sigma}_n$ then represent the contributions from a definite set of linked Goldstone diagrams. It has been noted in I, and explained in more detail elsewhere,[7] how these sets can be conveniently classified in terms of extended, generalized time-ordered tree diagrams, which branch both forwards and backwards in time.

We now take this opportunity to note that the normalization of the real-space amplitudes $\{S_n,S_n''\}$ and $\{\sigma_n,\bar{\sigma}_n\}$ implied by Eqs. (2.11)–(2.14), is chosen purely for convenience for present purposes. A comparison of the present equations with their formal and general counterparts in I should be made with great care for this reason. In particular, using Eq. (2.4b) of I, a comparison of Eqs. (3.11)–(3.16) of I with Eqs. (2.11)–(2.14) of the present paper, shows that each of the amplitudes $\{S_n,S_n''\}$ and $\{\sigma_n,\bar{\sigma}_n\}$ used in the present paper is a factor $(n!)^{1/2}$ greater than its counterpart in I. Nevertheless, many of the resulting equations appear *identical* in form here to their counterparts in I, *despite* this different normalization. This will arise in general due to the fact that each of the real-space amplitudes used in the present paper exhibits complete symmetry under permutation of its arguments. It is this symmetry which, for example, leads to the disappearance of the factor $(n!)^{-1}$ in Eqs. (2.19a) and (2.19b) as compared with its appearance in Eqs. (2.18a) and (2.18b) whence they were derived, and which ultimately makes Eqs. (2.19a) and (2.19b) here appear identical to their general counterparts, Eqs. (5.3) and (5.4) of I.

Finally, we note that it was shown in detail in I how to express, within the ECCM, the average-value functional of an arbitrary product of operators, in terms of the average-value functionals of the individual operators and their functional derivatives with respect to the basic amplitudes $\{\sigma_n,\bar{\sigma}_n\}$. In particular, we recall the especially important result for the expectation value of the commutator of an arbitrary pair of operators A and B,

$$\langle\Psi_0'|[A,B]|\Psi_0\rangle=i\{\bar{A},\bar{B}\}\ , \tag{2.20}$$

where the *generalized Poisson bracket* $\{\bar{A},\bar{B}\}$ is defined in our present normalization scheme as

$$i\{\bar{A},\bar{B}\}\equiv\sum_{n=1}^{\infty}\frac{1}{n!}\int dx_1\cdots\int dx_n\left[\frac{\delta\bar{A}}{\delta\sigma_n(x_1,\ldots,x_n;t)}\frac{\delta\bar{B}}{\delta\bar{\sigma}_n(x_1,\ldots,x_n;t)}-\frac{\delta\bar{A}}{\delta\bar{\sigma}_n(x_1,\ldots,x_n;t)}\frac{\delta\bar{B}}{\delta\sigma_n(x_1,\ldots,x_n;t)}\right]\ . \tag{2.21}$$

We stressed in I how Eq. (2.21) characterizes the fact that the ECCM may be viewed as an exact mapping of an arbitrary quantum many-body theory into the classical Hamiltonian mechanics for the many-body, classical (c-number) configuration-space amplitudes $\sigma_n(x_1,\ldots,x_n;t)$ and $\bar{\sigma}_n(x_1,\ldots,x_n;t)$. In turn, these may be mapped onto a set of generalized, classical many-body fields $\phi_n\equiv 2^{-1/2}(\sigma_n+\bar{\sigma}_n)$ and their canonically conjugate generalized momentum densities $\pi_n\equiv 2^{-1/2}i(\bar{\sigma}_n-\sigma_n)$. Of course, the ECCM is not the only mapping that achieves such a decomposition of a quantum many-body theory into a set of interacting nonlocal classical fields. Where it does seem to be unique is that the underlying amplitudes $\{\sigma_n,\bar{\sigma}_n\}$—a knowledge of which suffices to determine all physical quantities for the system—are all linked-cluster quantities, and hence are quasilocal in the sense of obeying the cluster property. This property is quite vital for later applications involving topological deformations, or where topological boundary conditions are imposed.

For ease of further notation, we shall henceforth usually suppress the time argument of our basic dynamical variables $\{\sigma_n,\bar{\sigma}_n\}$, which now completely characterize the system. Indeed, the time dependence of all dynamic variables will henceforth mostly be left implicit.

III. GAUGE INVARIANCE AND THE GAUGE FIELDS

We turn our attention now to an application of the ECCM techniques discussed above to a Bose liquid, with the basic aim of deriving the appropriate gauge-invariant hydrodynamical balance equations for such local observables as the number density, the current density, and the energy density. As usual, we seek to employ the standard Bogoliubov prescription[9–12] for the macroscopic occupation of the condensate by an explicit breaking of the underlying gauge symmetry which arises from the conservation of particle number. Technically, this is achieved by using the boson vacuum as our model state $|\Phi\rangle$, in which case the ECCM states of Eqs. (2.4a) and (2.4b) are not states of definite particle number. Particle-number conservation is then imposed by working not with the original many-body Hamiltonian $h_{(0)}$ for the fully interacting system but rather with the grand-canonical Hamiltonian $H_{(0)}\equiv h_{(0)}-\mu N$, where μ is the chemical potential and N the number operator. In the present case we consider a system of identical bosons, each of mass m and interacting via pairwise potentials,

$$h_{(0)}=-\frac{1}{2m}\sum_{j=1}^{N}\nabla_j^2+\sum_{i=1}^{N}\sum_{j<i}v(x_i-x_j)\ , \tag{3.1}$$

in units with $\hbar=1$.

The ECCM formulation as outlined in Sec. II immediately provides a theory capable of dealing with the general case of a spatially nonuniform and time-varying condensate, $\langle a_x \rangle \equiv \langle \Psi'(t) \mid a_x \mid \Psi(t) \rangle$. Indeed this condensate wave function $\langle a_x \rangle$ is precisely the one-body ECCM amplitude $\sigma_1(x)$, as follows from the definitions of Eqs. (2.4a) and (2.4b),

$$\langle a_x \rangle = \langle \Phi \mid e^{S''} e^{-S} a_x e^{S} \mid \Phi \rangle \ , \tag{3.2}$$

together with the definition of Eq. (2.11), which shows that

$$e^{-S} a_x e^{S} = a_x + [a_x, S] \ . \tag{3.3}$$

Finally, use of the relation $a_x \mid \Phi \rangle = 0$ shows that

$$\langle a_x \rangle = \langle \Phi \mid e^{S''} a_x S \mid \Phi \rangle = \sigma_1(x) \ , \tag{3.4}$$

where the last equality follows from the definition of Eq. (2.14).

Due to the underlying number conservation of the original Hamiltonian $h_{(0)}$, we ultimately wish to construct the theory in a gauge-invariant fashion. In this way we are led to consider[16] from the outset the coupling of the system to the external *gauge fields* ϕ and $\mathbf{A}$ (the scalar and vector potentials), and their transformation properties under local gauge transformations. Just as in standard electrodynamics we therefore study the Hamiltonian $H_{(0)} \rightarrow H$, where

$$H \equiv \sum_{j=1}^{N} \frac{1}{2m} [-i\nabla_j - \mathbf{A}(x_j)]^2 + \sum_{j=1}^{N} [\phi(x_j) - \mu] + \sum_{i=1}^{N} \sum_{j<i} v(x_i - x_j) \ . \tag{3.5}$$

The gauge fields are both space and time dependent, but in keeping with our notation the explicit time argument will usually be suppressed. In the notation of second quantization the Hamiltonian may be rewritten as

$$H = \frac{1}{2m} \int dr (\nabla_r a_r^\dagger) \cdot (\nabla_r a_r) + \frac{i}{2m} \int dr \ \mathbf{A}(r) \cdot [a_r^\dagger (\nabla_r a_r) - (\nabla_r a_r^\dagger) a_r] + \int dr \left[\phi(r) - \mu + \frac{1}{2m} \mathbf{A}^2(r) \right] a_r^\dagger a_r + \tfrac{1}{2} \int dr \int dr' v(r-r') a_r^\dagger a_{r'}^\dagger a_{r'} a_r \ . \tag{3.6}$$

Alternatively, we can display the explicit coupling of the external gauge fields to the system via the particle number density and canonical current density operators $\rho(r)$ and $\mathbf{j}(r)$, respectively,

$$\rho(r) \equiv a_r^\dagger a_r \ , \qquad \mathbf{j}(r) \equiv \lim_{r' \rightarrow r} \frac{i}{2m} (\nabla_r - \nabla_{r'}) a_r^\dagger a_{r'} \ , \tag{3.7}$$

by writing the Hamiltonian of Eq. (3.6) in the equivalent form,

$$H = H_{(0)} + \int dr \left[\left[\phi(r) + \frac{1}{2m} \mathbf{A}^2(r) \right] \rho(r) - \mathbf{A}(r) \cdot \mathbf{j}(r) \right] . \tag{3.8}$$

In the case of charged bosons (which we do not consider here), the necessity of the gauge-field description is apparent, since the charges couple to the electromagnetic fields through the Lorentz force. We wish to point out that the gauge-field description is also extremely useful in the case of neutral particles, since it allows a unified treatment of certain physically important coordinate transformations. We shall illustrate this immediately by considering pure displacements and pure rotations of the observer or of the system. If, in the original frame of some observer (0) a quantum-mechanical system is in some state $\mid s_0 \rangle$, it is well known[17] that in the frame of another observer (1), who is simply displaced by a constant vector $\mathbf{a}$ with respect to observer (0), the system will be described by the transformed wave function

$$\mid s \rangle = e^{i\mathbf{a} \cdot \mathbf{P}} \mid s_0 \rangle \ , \tag{3.9a}$$

where $\mathbf{P}$ is the total momentum operator which is the generator of space translations. Similarly if the observer (1) is simply rotated by an angle ϕ about an axis defined by the unit vector $\hat{\mathbf{n}}$ with respect to observer (0), the system will be described by the transformed wave function

$$\mid s \rangle = e^{i\phi \hat{\mathbf{n}} \cdot \mathbf{L}} \mid s_0 \rangle \ , \tag{3.9b}$$

where $\mathbf{L}$ is the total angular momentum operator which is the generator of rotations in space. If, to cover both cases, we use T to indicate the transformation operator, $\mid s \rangle = T \mid s_0 \rangle$, it is clear that if in the frame of the original observer (0), the system is governed by a Hamiltonian $H_{(0)}$,

$$H_{(0)} \mid s_0 \rangle = i \frac{\partial}{\partial t} \mid s_0 \rangle \ , \tag{3.10a}$$

then we may write for observer (1),

$$H \mid s \rangle = i \frac{\partial}{\partial t} \mid s \rangle \ , \tag{3.10b}$$

where the effective Hamiltonian for observer (1) is given by

$$H = T H_{(0)} T^{-1} + i \dot{T} T^{-1} \ . \tag{3.11}$$

Two particularly important examples are the cases of (a) uniform motion, $\mathbf{a} = \mathbf{V}_0 t$ in Eq. (3.9a), and (b) uniform rotation, $\hat{\mathbf{n}}\phi = \boldsymbol{\Omega} t$ in Eq. (3.9b), between observers (0) and (1). If the system has a Hamiltonian $H_{(0)}$ which is translationally invariant and rotationally invariant, so that $T H_{(0)} T^{-1} = H_{(0)}$ in both cases, these two cases are described, respectively, as

$$H = H_{(0)} - \mathbf{V}_0 \cdot \mathbf{P} \tag{3.12a}$$

and

$$H = H_{(0)} - \boldsymbol{\Omega} \cdot \mathbf{L} \ . \tag{3.12b}$$

In our own gauge-field description these two cases are

duplicated, respectively, by the choices

$$\mathbf{A}(r)=m\mathbf{V}_0,\quad \phi(r)=-\tfrac{1}{2}mV_0^2\ , \tag{3.13a}$$

and

$$\mathbf{A}(r)=m\boldsymbol{\Omega}\times\mathbf{r},\quad \phi(r)=-\tfrac{1}{2}m\,|\,\boldsymbol{\Omega}\times\mathbf{r}\,|^2\ . \tag{3.13b}$$

In the electromagnetic case, the second example of Eq. (3.13b) would just correspond to the well-known combination of crossed electric and magnetic fields that produces uniform rotational motion.

The real value of the gauge-invariant description becomes apparent where the observer (or, equivalently, the system) is neither in uniform translational motion nor in uniform rotation, but rather in a completely general state of motion. The use of general gauge fields can then be interpreted, in the light of the above examples, as providing differential or local Galilean transformations, where the (gauge-invariant) physical forces try to create local translational motions which vary from place to place within the system. It is clear that a proper hydrodynamical description of such systems must, for example, be able to distinguish the local hydrodynamical translational kinetic energy density from the intrinsic kinetic energy density in the local rest frame in a gauge-invariant fashion. In the remainder of this paper we shall show how such a complete hydrodynamical description of a condensed Bose system is provided by the ECCM whose framework we have already discussed.

IV. EQUATIONS OF MOTION FOR THE ECCM AMPLITUDES AND THE DENSITY MATRIX

In order to derive the explicit equations of motion for the basic ECCM amplitudes $\{\sigma_n,\tilde{\sigma}_n\}$ from the formal relations of Eq. (2.19), it is convenient to introduce the one- and two-body density matrices. The one-body density matrix is defined as usual by

$$\begin{aligned}&\bar{\rho}(r,r')=\bar{\rho}(r,r';t)\equiv\langle\Psi'(t)\,|\,\rho(r,r')\,|\,\Psi(t)\rangle\ ,\\&\rho(r,r')\equiv a_r^\dagger a_{r'}\ .\end{aligned} \tag{4.1}$$

By substituting from Eq. (2.4), it may be written as

$$\begin{aligned}\bar{\rho}(r,r')&=\langle\Phi\,|\,e^{S''}e^{-S}a_r^\dagger a_{r'}e^{S}\,|\,\Phi\rangle\\&=\langle\Phi\,|\,e^{S''}a_r^\dagger e^{-S''}e^{S''}e^{-S}a_{r'}e^{S}\,|\,\Phi\rangle\ ,\end{aligned} \tag{4.2}$$

where we have made use of Eq. (2.11). By making use of Eq. (3.3) and its counterpart,

$$e^{S''}a_r^\dagger e^{-S''}=a_r^\dagger+[S'',a_r^\dagger]\ , \tag{4.3}$$

together with the relations $\langle\Phi\,|\,a_r^\dagger=0=a_{r'}\,|\,\Phi\rangle$, Eq. (4.2) is readily rewritten as

$$\begin{aligned}\bar{\rho}(r,r')&=\langle\Phi\,|\,S''a_r^\dagger Ie^{S''}a_{r'}S\,|\,\Phi\rangle\\&=\langle\Phi\,|\,\tilde{\Sigma}a_r^\dagger Ia_{r'}\Sigma\,|\,\Phi\rangle\ ,\end{aligned} \tag{4.4}$$

where we have also used Eq. (2.15). Finally, inserting a resolution of the identity I of the form of Eq. (2.10) in the place so marked in Eq. (4.4) gives the explicit relation

$$\begin{aligned}\bar{\rho}(r,r')=\sum_{n=0}^{\infty}\frac{1}{n!}\int dx_1\cdots\int dx_n\tilde{\sigma}_{n+1}(r,x_1,\ldots,x_n)\\\times\sigma_{n+1}(r',x_1,\ldots,x_n)\ ,\end{aligned} \tag{4.5}$$

where we have used Eq. (2.14). Due to the cluster property which is obeyed by each of the amplitudes $\{\sigma_n,\tilde{\sigma}_n\}$, the one-body density matrix behaves simply in the limit of large separations as

$$\bar{\rho}(r,r')\to\tilde{\sigma}_1(r)\sigma_1(r')\quad\text{as}\ |\,\mathbf{r}-\mathbf{r}'\,|\to\infty\ , \tag{4.6}$$

thereby exhibiting the well-known behavior of off-diagonal long-range order,[18,19] typical of superfluid systems.

The two-body density matrix is similarly defined in the notation of Eqs. (2.7) and (2.8) as

$$\langle a_{r_1}^\dagger a_{r_2}^\dagger a_{r_3}a_{r_4}\rangle=\langle\Phi\,|\,\hat{a}_{r_1}^\dagger\hat{a}_{r_2}^\dagger I\hat{a}_{r_3}\hat{a}_{r_4}\,|\,\Phi\rangle\ , \tag{4.7}$$

which can again be rewritten, after a resolution of the identity I of the form of Eq. (2.10) as

$$\begin{aligned}&\langle a_{r_1}^\dagger a_{r_2}^\dagger a_{r_3}a_{r_4}\rangle\\&\quad=\sum_{n=0}^{\infty}\frac{1}{n!}\int dx_1\cdots\int dx_n\phi_{n+2}(r_1,r_2;x_1,\ldots,x_n)\\&\qquad\times\chi_{n+2}(r_3,r_4;x_1,\ldots,x_n)\ ,\end{aligned} \tag{4.8}$$

in terms of the *reduced subsystem amplitudes*,[5,7] defined as

$$\phi_{n+2}(r,r';x_1,\ldots,x_n)\equiv\langle\Phi\,|\,\hat{a}_r^\dagger\hat{a}_{r'}^\dagger a_{x_1}^\dagger\cdots a_{x_n}^\dagger\,|\,\Phi\rangle\ , \tag{4.9a}$$

$$\chi_{n+2}(r,r';x_1,\ldots,x_n)\equiv\langle\Phi\,|\,a_{x_1}\cdots a_{x_n}\hat{a}_r\hat{a}_{r'}\,|\,\Phi\rangle\ . \tag{4.9b}$$

Explicit evaluations of Eqs. (4.9a) and (4.9b) for the reduced subsystem amplitudes in terms of the basic ECCM amplitudes $\{\sigma_n,\tilde{\sigma}_n\}$ are given in Appendix A. The final results are given by Eqs. (A7), (A18), and (A19). An alternative exact representation of the two-body density matrix is given in Appendix B using the functional derivative technique for the expectation value of the product of two one-body operators, as discussed in I.

In terms of the diagonal elements of the two-body density operator,

$$D(r,r')=D(r,r';t)\equiv\langle a_r^\dagger a_{r'}^\dagger a_{r'}a_r\rangle\ , \tag{4.10}$$

we can evaluate the average potential energy of the system as

$$\bar{V}=\bar{V}[\sigma_n,\tilde{\sigma}_n]=\tfrac{1}{2}\int dr\int dr'v(r-r')D(r,r')\ . \tag{4.11}$$

Now, using the explicit Hamiltonian of Eq. (3.6) and the one-body density matrix of Eq. (4.5), we have

$$\bar{H}=\sum_{n=0}^{\infty}\frac{1}{n!}\int dr\int dx_1\cdots\int dx_n\left[\frac{1}{2m}\nabla_r\tilde{\sigma}_{n+1}(r,x_1,\ldots,x_n)\cdot\nabla_r\sigma_{n+1}(r,x_1,\ldots,x_n)\right.$$
$$+\frac{i}{2m}\tilde{\sigma}_{n+1}(r,x_1,\ldots,x_n)\,\mathbf{A}(r)\cdot\nabla_r\sigma_{n+1}(r,x_1,\ldots,x_n)$$
$$-\frac{i}{2m}\sigma_{n+1}(r,x_1,\ldots,x_n)\,\mathbf{A}(r)\cdot\nabla_r\tilde{\sigma}_{n+1}(r,x_1,\ldots,x_n)$$
$$\left.+\left[\phi(r)-\mu+\frac{1}{2m}\mathbf{A}^2(r)\right]\sigma_{n+1}(r,x_1,\ldots,x_n)\tilde{\sigma}_{n+1}(r,x_1,\ldots,x_n)\right]+\bar{V}\ . \tag{4.12}$$

By straightforward partial integration, Eq. (4.12) may be expressed equivalently in either of the forms

$$\bar{H}=\sum_{n=0}^{\infty}\frac{1}{n!}\int dr\int dx_1\cdots\int dx_n\tilde{\sigma}_{n+1}(r,x_1,\ldots,x_n)[h(r)\sigma_{n+1}(r,x_1,\ldots,x_n)]+\bar{V}$$
$$=\sum_{n=0}^{\infty}\frac{1}{n!}\int dr\int dx_1\cdots\int dx_n\sigma_{n+1}(r,x_1,\ldots,x_n)[\tilde{h}(r)\tilde{\sigma}_{n+1}(r,x_1,\ldots,x_n)]+\bar{V} \tag{4.13}$$

in terms of the reduced one-body Hamiltonians defined as

$$h(r)\equiv-\frac{1}{2m}\nabla_r^2+\frac{i}{m}\mathbf{A}(r)\cdot\nabla_r+\frac{i}{2m}[\nabla_r\cdot\mathbf{A}(r)]$$
$$+\frac{1}{2m}\mathbf{A}^2(r)+\phi(r)-\mu \tag{4.14a}$$

and

$$\tilde{h}(r)\equiv-\frac{1}{2m}\nabla_r^2-\frac{i}{m}\mathbf{A}(r)\cdot\nabla_r-\frac{i}{2m}[\nabla_r\cdot\mathbf{A}(r)]$$
$$+\frac{1}{2m}\mathbf{A}^2(r)+\phi(r)-\mu\ . \tag{4.14b}$$

Using Eqs. (2.19) and (4.13), it is then straightforward to derive the exact equations of motion for the ECCM amplitudes as

$$i\frac{d}{dt}\sigma_n(x_1,\ldots,x_n)=\sum_{j=1}^{n}h(x_j)\sigma_n(x_1,\ldots,x_n)$$
$$+\frac{\delta\bar{V}}{\delta\tilde{\sigma}_n(x_1,\ldots,x_n)}\ , \tag{4.15a}$$

$$-i\frac{d}{dt}\tilde{\sigma}_n(x_1,\ldots,x_n)=\sum_{j=1}^{n}\tilde{h}(x_j)\tilde{\sigma}_n(x_1,\ldots,x_n)$$
$$+\frac{\delta\bar{V}}{\delta\sigma_n(x_1,\ldots,x_n)}\ , \tag{4.15b}$$

where we have made use of the complete symmetry of the amplitudes $\{\sigma_n,\tilde{\sigma}_n\}$ under permutations of their arguments, as in the discussion below Eqs. (2.19a) and (2.19b). For the purposes of the remainder of this paper we shall not need the explicit expressions for the functional derivatives of the average-value functional $\bar{V}$ in Eqs. (4.15a) and (4.15b). We point out, however, that they could be found quite straightforwardly using the explicit expressions obtained in either of the Appendixes. Finally, we also note that Eqs. (4.14) and (4.15) may be regarded as an exact coupled hierarchy of nonlinear equations which generalize the approximate Gross-Pitaevskii[13,14] nonlinear equations for weakly interacting condensed Bose liquids. In fact, the Gross-Pitaevskii equations are precisely obtained as our SUB1 approximation, in which all of the amplitudes σ_n and $\tilde{\sigma}_n$ with $n>1$ are set to zero. This results in self-consistent time-dependent Hartree equations for the amplitudes $\sigma_1(r)$ and $\tilde{\sigma}_1(r)$. The Gross-Pitaevskii equations are then just the equilibrium (in time) counterparts of these equations, in which the interparticle potential is further replaced by a repulsive δ-function potential.

The basic equations of motion (4.14) and (4.15) can now be used to construct the equations of motion for average values of arbitrary operators. Of particular interest is the one-body density matrix, for which we can use the representation of Eq. (4.5). A few straightforward integrations by parts and some rearrangements of terms easily leads to the result

$$\frac{\partial}{\partial t}\bar{\rho}(r,r')=\frac{i}{2m}(\nabla_{r'}^2-\nabla_r^2)\bar{\rho}(r,r')+\frac{1}{m}[\mathbf{A}(r)\cdot\nabla_r+\mathbf{A}(r')\cdot\nabla_{r'}]\bar{\rho}(r,r')+i\left[\phi(r)-\phi(r')+\frac{1}{2m}\{\mathbf{A}^2(r)-\mathbf{A}^2(r')\}\right]\bar{\rho}(r,r')$$
$$+\frac{1}{2m}[\{\nabla_r\cdot\mathbf{A}(r)\}+\{\nabla_{r'}\cdot\mathbf{A}(r')\}]\bar{\rho}(r,r')+iC(r,r')\ , \tag{4.16}$$

where the function $C(r,r')$ is defined as

$$C(r,r')\equiv\sum_{n=0}^{\infty}\frac{1}{n!}\int dx_1\cdots\int dx_n\left[\frac{\delta\bar{V}}{\delta\sigma_{n+1}(r,x_1,\ldots,x_n)}\sigma_{n+1}(r',x_1,\ldots,x_n)-\frac{\delta\bar{V}}{\delta\tilde{\sigma}_{n+1}(r',x_1,\ldots,x_n)}\tilde{\sigma}_{n+1}(r,x_1,\ldots,x_n)\right]. \tag{4.17}$$

By making use of the relations

$$\begin{aligned}\delta\bar{\rho}(r,r')/\delta\tilde{\sigma}_n(x_1,\ldots,x_n)&=\sum_{i=1}^{n}\sigma_n(x_1,\ldots,x_{i-1},r',x_{i+1},\ldots,x_n)\delta(x_i-r)\,,\\ \delta\bar{\rho}(r,r')/\delta\sigma_n(x_1,\ldots,x_n)&=\sum_{i=1}^{n}\tilde{\sigma}_n(x_1,\ldots,x_{i-1},r,x_{i+1},\ldots,x_n)\delta(x_i-r')\,,\end{aligned} \tag{4.18}$$

which follow quite straightforwardly from Eq. (4.5), it is not difficult to show that Eq. (4.17) may be rewritten as

$$C(r,r')=\sum_{n=1}^{\infty}\frac{1}{n!}\int dx_1\cdots\int dx_n\left[\frac{\delta\bar{V}}{\delta\sigma_n(x_1,\ldots,x_n)}\frac{\delta\bar{\rho}(r,r')}{\delta\tilde{\sigma}_n(x_1,\ldots,x_n)}-\frac{\delta\bar{V}}{\delta\tilde{\sigma}_n(x_1,\ldots,x_n)}\frac{\delta\bar{\rho}(r,r')}{\delta\sigma_n(x_1,\ldots,x_n)}\right]. \tag{4.19}$$

A comparison of Eq. (4.19) with Eq. (2.21) shows that the function $C(r,r')$ may be expressed in terms of a generalized Poisson bracket as

$$C(r,r')=i\{\bar{V},\bar{\rho}(r,r')\}\,, \tag{4.20}$$

which is important for later purposes.

V. THE ONE-BODY DENSITY MATRIX AND GAUGE TRANSFORMATIONS

We now turn our attention to the basic reason for the introduction of the gauge fields $\phi(r)$ and $\mathbf{A}(r)$. Thus, we know that under a local gauge transformation the Schrödinger wave function of an N-body system changes as

$$\Psi(x_1,\ldots,x_N)\rightarrow\Psi'(x_1,\ldots,x_N)=\exp\left[-i\sum_{j=1}^{N}\Lambda(x_j,t)\right]\Psi(x_1,\ldots,x_N)\,, \tag{5.1}$$

in such a way that it simply acquires a space-time–dependent phase factor via a phase-function $\Lambda(r,t)\equiv\Lambda(r)$, where the time dependence, as usual, will be left implicit. The time evolution of the transformed field Ψ' is then readily seen from Eqs. (2.3) and (3.5) to follow a Hamiltonian of precisely the same form but with correspondingly transformed gauge fields,

$$\begin{aligned}&\mathbf{A}\rightarrow\mathbf{A}'=\mathbf{A}-\nabla\Lambda\,,\\ &\phi\rightarrow\phi'=\phi+\partial\Lambda/\partial t\,.\end{aligned} \tag{5.2}$$

Within the ECCM the local gauge transformation may equivalently be completely specified by its mode of action on the basic linked-cluster amplitudes,

$$\begin{aligned}\sigma_n(x_1,\ldots,x_n)&\rightarrow\sigma_n'(x_1,\ldots,x_n)=\exp\left[-i\sum_{j=1}^{n}\Lambda(x_j)\right]\sigma_n(x_1,\ldots,x_n)\,,\\ \tilde{\sigma}_n(x_1,\ldots,x_n)&\rightarrow\tilde{\sigma}_n'(x_1,\ldots,x_n)=\exp\left[+i\sum_{j=1}^{n}\Lambda(x_j)\right]\tilde{\sigma}_n(x_1,\ldots,x_n)\,.\end{aligned} \tag{5.3}$$

It is immediately clear that the diagonal terms of the one-body density matrix $\bar{\rho}(r,r)\equiv\bar{\rho}(r)$ and of the two-body density matrix $D(r,r')$, and hence also the average-value functional $\bar{V}[\sigma_n,\tilde{\sigma}_n]$ of the potential energy, are invariant under gauge transformations of the form of Eq. (5.3). The basic reason for this is that in the expressions (4.5) and (4.8)–(4.10) for these quantities, every amplitude $\tilde{\sigma}_n$ or ϕ_n, respectively, that appears, is always multiplied by a corresponding amplitude σ_n or χ_n, respectively, with exactly the same arguments. Each phase factor introduced by the gauge transformation is then immediately matched with its complex conjugate to produce a null change. An immediate consequence of this is that the change in $\bar{V}$ must identically vanish in any gauge transformation, and in particular we have $\delta\bar{V}=0$ for an arbitrary infinitesimal gauge transformation with phase function $\delta\Lambda$. By the usual rules of partial differentiation, and again using the complete symmetry under permutations of the arguments of the basic amplitudes $\{\sigma_n,\tilde{\sigma}_n\}$, an infinitesimal $\delta\bar{V}$ may be expressed as

$$\delta\bar{V}=\sum_{n=1}^{\infty}\frac{1}{n!}\int dx_1\cdots\int dx_n\left[\frac{\delta\bar{V}}{\delta\sigma_n(x_1,\ldots,x_n)}\delta\sigma_n(x_1,\ldots,x_n)+\frac{\delta\bar{V}}{\delta\tilde{\sigma}_n(x_1,\ldots,x_n)}\delta\tilde{\sigma}_n(x_1,\ldots,x_n)\right]. \tag{5.4}$$

Indeed, this may be viewed as the definition of the functional derivatives which is consistent with the earlier discussion in Secs. II and IV. For an infinitesimal gauge transformation with phase function $\delta\Lambda(r)$, Eq. (5.3) gives

$$\delta\sigma_n(x_1,\ldots,x_n)=-i\sigma_n(x_1,\ldots,x_n)\sum_{j=1}^{n}\delta\Lambda(x_j)\ ,$$
$$\delta\bar{\sigma}_n(x_1,\ldots,x_n)=+i\bar{\sigma}_n(x_1,\ldots,x_n)\sum_{j=1}^{n}\delta\Lambda(x_j)\ . \tag{5.5}$$

Substituting Eq. (5.5) into Eq. (5.4), and again using the permutation symmetry of the amplitudes $\{\sigma_n,\bar{\sigma}_n\}$, then readily gives the result

$$\delta\bar{V}=-i\int dr\, C(r,r)\delta\Lambda(r)\ , \tag{5.6}$$

where we have used the definition (4.17) of the function $C(r,r')$. Since $\delta\bar{V}=0$ for all $\delta\Lambda(r)$, we then immediately have

$$C(r,r)=0\ . \tag{5.7}$$

We shall subsequently also require the detailed behavior of the function $C(r,r')$ as the two arguments $\mathbf{r},\mathbf{r}'$ become close to each other. This is most readily obtained from Eq. (4.20) and the general results of Eqs. (2.20) and (2.21) which relate the generalized Poisson brackets to the expectation values of the corresponding operator commutator. We thus have

$$C(r,r')=\tfrac{1}{2}\int dx\int dy\, v(x-y)\langle[a_x^\dagger a_y^\dagger a_y a_x,a_r^\dagger a_{r'}]\rangle$$
$$=\int dx[v(r-x)-v(r'-x)]\langle a_x^\dagger a_r^\dagger a_{r'}a_x\rangle\ , \tag{5.8}$$

where in the second equality we have used the basic boson commutation relations (2.9) and the implicit rotational invariance of the two-body potential, $v(r-r')=v(|\mathbf{r}-\mathbf{r}'|)=v(r'-r)$. We note that the special result (5.7) also follows immediately from the general relation of Eq. (5.8).

We note at this point that the result of Eq. (5.8) could have been obtained much more directly by starting from the Heisenberg equation of motion for the density operator $\rho(r,r')$. Then, upon taking the average value we would obtain the equation of motion (4.16) for the density matrix $\bar{\rho}(r,r')$ but with the term $C(r,r')$ directly in the form of Eq. (5.8). In the present context this extremely convenient property can be viewed as providing a double check both on the derivation of Eq. (4.16) from the equations of motion (4.15) of the basic ECCM amplitudes $\{\sigma_n,\tilde{\sigma}_n\}$ and indeed on the consistency of the general theory presented in I and reviewed here in Sec. II. We take pains to stress, however, that the result of Eq. (5.8) is itself completely derivable from the defining relation of Eq. (4.17). We would simply need to use the relationship (4.11) for $\bar{V}$ and the expression for the diagonal terms of the two-body density matrix $D(r,r')$ from Eqs. (4.8) and (4.10), together with the explicit results in Appendix A for the reduced subsystem amplitudes χ and ϕ in terms of the linked-cluster amplitudes $\{\sigma_n,\bar{\sigma}_n\}$. Equivalent results could also be obtained using the decomposition in Appendix B. In these cases, however, the direct method is rather cumbersome [but the dedicated reader may persuade himself that these derivations also lead to Eq. (5.8)]. As seen here, one can use the freedom to exploit either method, to great advantage.

We return now to the equation of motion (4.16) for $\bar{\rho}(r,r')$. Since we are ultimately interested in deriving the hydrodynamical balance (or local conservation) equations for the various local observables of interest, we shall need to take the limit as $\mathbf{r}'\to\mathbf{r}$. Equation (5.8) will enable us to do this for the term $C(r,r')$, but in light of the derivative terms in Eq. (4.16) we still need to investigate the nondiagonal terms $\bar{\rho}(r,r')$ in the vicinity of the diagonal $\mathbf{r}'\to\mathbf{r}$. For these purposes it is convenient to change to relative and center-of-mass coordinates,

$$\mathbf{R}\equiv\tfrac{1}{2}(\mathbf{r}+\mathbf{r}'),\quad \boldsymbol{\xi}\equiv\mathbf{r}-\mathbf{r}'\ , \tag{5.9}$$

in terms of which the spatial derivatives in Eq. (4.16) become

$$\nabla_r=\tfrac{1}{2}\nabla_R+\nabla_\xi\ ,\quad \nabla_{r'}=\tfrac{1}{2}\nabla_R-\nabla_\xi\ . \tag{5.10}$$

In this work we shall be interested in expanding Eq. (4.16) to include terms up to second order in $\boldsymbol{\xi}$, and it will therefore turn out to be necessary to expand the density matrix up to third-order terms. We define the coefficients in this Taylor expansion by the relation

$$\bar{\rho}(r,r')\equiv\bar{\rho}(R\mid\xi)$$
$$=\bar{\rho}(R)+\beta^a(R)\xi^a+\tfrac{1}{2}\gamma^{ab}(R)\xi^a\xi^b$$
$$+\tfrac{1}{6}\delta^{abc}(R)\xi^a\xi^b\xi^c+O(\xi^4)\ , \tag{5.11}$$

where $\bar{\rho}(R)=\bar{\rho}(R,R)$ is just the number density at R, and the superscripts a,b,c, etc., are Cartesian three-vector indices. The convention of summation over repeated indices is implied in Eq. (5.11) and is used consistently henceforth. We note that the tensor coefficients $\gamma^{ab},\delta^{abc},\ldots$ are all completely symmetric under arbitrary permutations of their indices.

From the Taylor theorem, the first-order coefficient $\beta^a(R)$ may be written as

$$\beta^a(R)\equiv\frac{\partial}{\partial\xi^a}\bar{\rho}(R\mid\xi)\bigg|_{\xi=0}$$
$$=\tfrac{1}{2}\lim_{r'\to r}(\nabla_r^a-\nabla_{r'}^a)\bar{\rho}(r,r')=-im j^a(R)\ , \tag{5.12}$$

where we have used Eq. (5.10) and where $\mathbf{j}(R)$ is just the local canonical current density [cf. Eq. (3.7)]. It should be quite apparent that just as the canonical current density, and hence the vector β^a, is not gauge invariant, so nor are the higher tensor coefficients $\gamma^{ab},\delta^{abc},\ldots$. In order to find the most convenient invariant combinations of each order, we use the transformation property of the density matrix under the gauge transformation (5.3),

$$\bar{\rho}(r,r')\to\bar{\rho}'(r,r')=e^{i[\Lambda(r)-\Lambda(r')]}\bar{\rho}(r,r')\ , \tag{5.13}$$

which follows immediately from Eq. (4.5); and hence

$$\ln\bar{\rho}'(R\mid\xi)=\ln\bar{\rho}(R\mid\xi)+i\xi^a(\partial^a\Lambda)$$
$$+\frac{i}{24}\xi^a\xi^b\xi^c(\partial^a\partial^b\partial^c\Lambda)+O(\xi^5)\ , \tag{5.14}$$

where $\partial^a\Lambda \equiv \partial\Lambda/\partial R^a$, as usual. In anticipation of the final result we expand $\ln\bar{\rho}$ in powers of ξ, up to the third, in the following specific form:

$$\ln[\bar{\rho}(R \mid \xi)/\bar{\rho}(R)] = -i\xi^a\left[A^a+\frac{m}{\bar{\rho}}J^a\right]-\frac{m^2}{2\bar{\rho}}\xi^a\xi^b\Gamma^{ab} + \frac{i}{3}\xi^a\xi^b\xi^c\left[-\tfrac{1}{24}(\partial^a\partial^b A^c+\partial^b\partial^c A^a+\partial^c\partial^a A^b) + \frac{m^2}{\bar{\rho}}\Delta^{abc}\right]+O(\xi^4)\ . \tag{5.15}$$

A straightforward comparison between Eqs. (5.14) and (5.15) of terms of comparable order shows

$$A'^a+\frac{m}{\bar{\rho}}J'^a = A^a+\frac{m}{\bar{\rho}}J^a-\partial^a\Lambda\ , \tag{5.16a}$$

$$\Gamma'^{ab}=\Gamma^{ab}\ , \tag{5.16b}$$

$$-\tfrac{1}{24}(\partial^a\partial^b A'^c+\partial^b\partial^c A'^a+\partial^c\partial^a A'^b)+\frac{m^2}{\bar{\rho}}\Delta'^{abc} = -\tfrac{1}{24}(\partial^a\partial^b A^c+\partial^b\partial^c A^a+\partial^c\partial^a A^b) + \frac{m^2}{\bar{\rho}}\Delta^{abc}+\tfrac{1}{8}\partial^a\partial^b\partial^c\Lambda\ . \tag{5.16c}$$

A combination of Eqs. (5.16) with the transformation rule of Eq. (5.2) for the vector potential then readily shows that the tensors $J^a(R)$, $\Gamma^{ab}(R)$, and $\Delta^{abc}(R)$ defined by Eq. (5.15) are gauge invariant, namely,

$$J'^a=J^a,\quad \Gamma'^{ab}=\Gamma^{ab},\quad \Delta'^{abc}=\Delta^{abc}\ . \tag{5.17}$$

Finally, a comparison of Eqs. (5.11) and (5.15) shows the connections between the various expansion coefficients,

$$J^a=j^a-\frac{\bar{\rho}}{m}A^a\ , \tag{5.18a}$$

$$\Gamma^{ab}=-\frac{1}{m^2}\gamma^{ab}-\frac{1}{\bar{\rho}}j^aj^b\ , \tag{5.18b}$$

$$\Delta^{abc}=\frac{1}{2im^2}\delta^{abc}+\frac{1}{2m\bar{\rho}}(j^a\gamma^{bc}+j^b\gamma^{ca}+j^c\gamma^{ab}) + \frac{m}{\bar{\rho}^2}j^aj^bj^c+\frac{\bar{\rho}}{24m^2}(\partial^a\partial^b A^c+\partial^b\partial^c A^a+\partial^c\partial^a A^b)\ . \tag{5.18c}$$

We remind the reader that all of the coefficients in Eqs. (5.18a)—(5.18c) are functions of position and of time. We also note that Eq. (5.18a) expresses the true particle current density J in terms of the canonical current density $\mathbf{j}$ in the usual fashion.

After these preliminaries we are now ready to expand the equation of motion (4.16) for $\bar{\rho}(R \mid \xi)$ up to second-order terms. The various terms not involving the potential $\bar{V}$ are rather straightforwardly expanded, using Eqs. (5.9)–(5.12), as

$$\frac{\partial}{\partial t}\bar{\rho}(r,r')=\frac{\partial\bar{\rho}}{\partial t}-im\xi^a\frac{\partial j^a}{\partial t}+\tfrac{1}{2}\xi^a\xi^b\frac{\partial\gamma^{ab}}{\partial t}+O(\xi^3)\ , \tag{5.19a}$$

$$\frac{i}{2m}[\nabla_{r'}^2-\nabla_r^2]\bar{\rho}(r,r') = -\partial^a j^a-\frac{i}{m}\xi^a(\partial^b\gamma^{ab})-\frac{i}{2m}\xi^a\xi^b(\partial^c\delta^{abc})+O(\xi^3)\ , \tag{5.19b}$$

$$\frac{1}{m}[\mathbf{A}(r)\cdot\nabla_r+\mathbf{A}(r')\cdot\nabla_{r'}]\bar{\rho}(r,r') = \frac{1}{m}A^a(\partial^a\bar{\rho})-i\xi^a[A^b(\partial^b j^a)+(\partial^a A^b)j^b] + \tfrac{1}{2}\xi^a\xi^b\frac{1}{m}[A^c(\partial^c\gamma^{ab})+\tfrac{1}{4}(\partial^a\partial^b A^c)(\partial^c\bar{\rho}) + (\partial^a A^c)\gamma^{bc}+(\partial^b A^c)\gamma^{ac}]+O(\xi^3)\ ; \tag{5.19c}$$

$$i\left[\phi(r)-\phi(r')+\frac{1}{2m}[\mathbf{A}^2(r)-\mathbf{A}^2(r')]\right]\bar{\rho}(r,r') = i\xi^a\bar{\rho}\left[\partial^a\phi+\frac{1}{m}A^b(\partial^a A^b)\right] + \tfrac{1}{2}\xi^a\xi^b\{j^a[m\partial^b\phi+A^c(\partial^b A^c)] + j^b[m\partial^a\phi+A^c(\partial^a A^c)]\}+O(\xi^3)\ , \tag{5.19d}$$

$$\frac{1}{2m}\{[\nabla_r\cdot\mathbf{A}(r)]+[\nabla_{r'}\cdot\mathbf{A}(r')]\}\bar{\rho}(r,r') = \frac{\bar{\rho}}{m}\partial^a A^a-i\xi^a[j^a(\partial^b A^b)] + \tfrac{1}{2}\xi^a\xi^b\left[\frac{1}{m}\gamma^{ab}(\partial^c A^c)+\frac{\bar{\rho}}{4m}\partial^a\partial^b\partial^c A^c\right]+O(\xi^3)\ . \tag{5.19e}$$

The final term in Eq. (4.16), which involves the two-body forces, is best evaluated, up to the terms of same order in ξ, from Eq. (5.8). We thus find

$$C(r,r')=\int dx[v(R-x+\tfrac{1}{2}\xi)-v(R-x-\tfrac{1}{2}\xi)]\langle a_x^\dagger a^\dagger_{R+\xi/2}a_{R-\xi/2}a_x\rangle = \xi^a\int dx[\partial^a v(R-x)]\langle a_x^\dagger a_R^\dagger a_R a_x\rangle - im\xi^a\xi^b\int dx[\partial^a v(R-x)]\langle a_x^\dagger j^b(r)a_x\rangle+O(\xi^3)\ , \tag{5.20}$$

where $j^b(R)$ is simply the canonical current density operator of Eq. (3.7). This expression is most conveniently reexpressed in terms of the following defined quantities,

$$\mathbf{F}_{\rm int}(r)\equiv-\frac{1}{\bar{\rho}(r)}\int dx[\nabla_r v(r-x)]D(r,x)\ , \tag{5.21}$$

where $D(r,x)$ is the diagonal piece of the two-body density matrix as specified previously in Eq. (4.10); and

$$W^{ab}(r)\equiv-\frac{1}{\bar{\rho}(r)}\int dx\left[\frac{\partial v(r-x)}{\partial r^a}\langle a_x^\dagger J^b(r)a_x\rangle+\frac{\partial v(r-x)}{\partial r^b}\langle a_x^\dagger J^a(r)a_x\rangle\right], \tag{5.22}$$

where $\mathbf{J}(r)$ is the gauge-invariant total current density operator, given by analogy with Eqs. (3.7) and (5.18a) as

$$\mathbf{J}(r)\equiv-\frac{i}{2m}[a_r^\dagger(\nabla_r a_r)-(\nabla_r a_r^\dagger)a_r]-\frac{1}{m}\mathbf{A}(r)a_r^\dagger a_r\ . \tag{5.23}$$

From our earlier discussion it is clear that both $\mathbf{F}_{\rm int}(r)$ and $W^{ab}(r)$ are gauge-invariant entities, in terms of which the remaining term in the equation of motion (4.16) for $\bar{\rho}(r,r')$ may be expanded as

$$iC(r,r')=-i\xi^a\bar{\rho}F^a_{\rm int}-\tfrac{1}{2}\xi^a\xi^b\bar{\rho}[A^aF^b_{\rm int}+A^bF^a_{\rm int}+mW^{ab}]+O(\xi^3)\ . \tag{5.24}$$

Finally, after insertion of Eqs. (5.19a)–(5.19e) and (5.24) into Eq. (4.16), a comparison of the coefficients of the terms of zeroth, first and second order in ξ, yields, respectively,

$$\frac{\partial\bar{\rho}}{\partial t}=-\partial^a j^a+\frac{1}{m}A^a(\partial^a\bar{\rho})+\frac{1}{m}\bar{\rho}(\partial^aA^a)\ , \tag{5.25}$$

$$\frac{\partial j^a}{\partial t}=\frac{1}{m^2}\partial^b\gamma^{ab}+\frac{1}{m}[(\partial^aA^b)j^b+A^b(\partial^bj^a)]-\frac{\bar{\rho}}{m}[\partial^a\phi+\frac{1}{m}A^b(\partial^aA^b)]+\frac{1}{m}j^a(\partial^bA^b)+\frac{\bar{\rho}}{m}F^a_{\rm int}\ , \tag{5.26}$$

and

$$\frac{\partial\gamma^{ab}}{\partial t}=-\frac{i}{m}\partial^c\delta^{abc}+\frac{1}{m}[\gamma^{ac}(\partial^bA^c)+\gamma^{bc}(\partial^aA^c)+\gamma^{ab}(\partial^cA^c)+A^c(\partial^c\gamma^{ab})]$$
$$+j^a[m\partial^b\phi+A^c(\partial^bA^c)]+j^b[m\partial^a\phi+A^c(\partial^aA^c)]+\frac{1}{4m}\partial^c(\bar{\rho}\partial^a\partial^bA^c)-\bar{\rho}[A^aF^b_{\rm int}+A^bF^a_{\rm int}+mW^{ab}]\ . \tag{5.27}$$

In Sec. VI we shall show that Eqs. (5.25)–(5.27) represent the hydrodynamical balance equations for the most important local quantities of physical interest. Before doing so, however, it is worthwhile to discuss the physical meaning of the gauge-invariant coefficients introduced above in connection with the terms in the equation of motion involving the two-body interactions. From the definition of Eq. (5.21), it is clear that $\mathbf{F}_{\rm int}(r)$ is the average force per particle at space point r due to the (internal) interparticle pairwise forces in the presence of correlations. Similarly, from the definition of Eq. (5.22) we recognize the gauge-invariant velocity field $\mathbf{u}(r)$,

$$\mathbf{u}(r)\equiv\mathbf{J}(r)/\bar{\rho}(r)\ . \tag{5.28}$$

The coefficient $W^{ab}(r)$ thus represents the (symmetrized) velocity-force correlation function. The trace $W^{aa}(r)$ thus represents the average increase of the internal kinetic energy per particle and per unit time at space point r, due to the pairwise interparticle forces.

VI. HYDRODYNAMICAL BALANCE EQUATIONS

We are now ready to analyze the physical content of Eqs. (5.25)–(5.27), and to show thereby that our ECCM description based on the equations of motion for the amplitudes $\{\sigma_n,\bar{\sigma}_n\}$ provides a complete and concise hydrodynamics for the zero-temperature interacting condensed Bose liquid.

A. The current continuity equation

Expressing Eq. (5.25) in terms of the (gauge-invariant) true current density $\mathbf{J}(r,t)$, we find the familiar form,

$$\frac{\partial\bar{\rho}}{\partial t}+\nabla\cdot\mathbf{J}=0\ , \tag{6.1}$$

of the current continuity equation. Equation (6.1) is simply the local form of the global conservation law, $d\bar{N}/dt=0$, for particle number, the correct imposition of which has been our main motivation for the introduction of the external gauge fields $\phi(r,t)$ and $\mathbf{A}(r,t)$. It is particularly important to point out that not only is Eq. (6.1) valid, as it must be, in the exact untruncated formalism, but is is also true in the usual approximation schemes. Of course, to put the ECCM to practical use such approximations are always necessary. A typical truncation scheme is the so-called SUBn scheme in which the linked-cluster amplitudes $\{\sigma_m,\bar{\sigma}_m\}$ with $m>n$ are set to zero, and the remaining coupled equations of motion (2.19a) and (2.19b) for $\{\sigma_i,\bar{\sigma}_i\}$ with $i\le n$ are solved. It should be immediately clear from our derivation of Eq. (5.25), which was based on Eq. (4.16) and the relation (4.5), that the current continuity equation also holds at every SUBn level of approximation.

B. Equation of motion for the momentum density

We turn now to the first-order (in ξ^a) equation (5.26), and reexpress it in terms of the gauge-invariant quantities J^a and Γ^{ab} from Eqs. (5.18a) and (5.18b) rather than the noninvariant quantities j^a and γ^{ab}. Making use of the current continuity equation (6.1) to rewrite the term $\partial\bar{\rho}/\partial t$ that arises from this procedure, it is then not difficult to show that Eq. (5.26) may be equivalently writ-

ten as

$$\frac{\partial J^a}{\partial t}+\partial^b\left[\frac{1}{\bar{\rho}}J^aJ^b\right]=\frac{\bar{\rho}}{m}F^a\ , \tag{6.2}$$

where $F^a(R)$ has the interpretation as the total average force per particle at point R, composed of three pieces,

$$F^a(R)\equiv F^a_{\rm int}(R)+F^a_{\rm ext}(R)+F^a_{\rm kin}(R)\ . \tag{6.3}$$

The term $F^a_{\rm int}$ has already been explained to be the average force per particle due to the internal interparticle forces. Similarly $F^a_{\rm ext}$ is the external force per particle due to the gauge fields, and it has the familiar Lorentz form

$$\mathbf{F}_{\rm ext}\equiv\mathbf{E}+\mathbf{u}\times\mathbf{B}\ , \tag{6.4}$$

where $\mathbf{u}$ is the velocity field of Eq. (5.28) and the fields $\mathbf{E}$ and $\mathbf{B}$ are defined in terms of the gauge fields ϕ and $\mathbf{A}$ as

$$\begin{aligned}&\mathbf{B}\equiv\nabla\times\mathbf{A}\ ,\\&\mathbf{E}\equiv-\nabla\phi-\partial\mathbf{A}/\partial t\ ,\end{aligned} \tag{6.5}$$

exactly as in electrodynamics. Again, just as in electrodynamics, the fields $\mathbf{E}$ and $\mathbf{B}$ so defined are invariant under gauge transformations of the type defined in Eq. (5.2). Finally, the term $\mathbf{F}_{\rm kin}$ in Eq. (6.3) is defined as

$$F^a_{\rm kin}\equiv-\frac{m}{\bar{\rho}}\partial^b\Gamma^{ab}\ , \tag{6.6}$$

and is hence proportional to the divergence of the kinetic stress tensor Γ^{ab}, which is itself proportional to the gauge-invariant second-order cumulant coefficient in the expansion of the logarithm of the one-body distribution function,

$$\Gamma^{ab}(R)=-\frac{\bar{\rho}(R)}{m^2}\frac{\partial^2}{\partial\xi^a\partial\xi^b}\times\left[\ln\left[\frac{\bar{\rho}(R+\frac{1}{2}\xi,R-\frac{1}{2}\xi)}{\bar{\rho}(R)}\right]\right]\Bigg|_{\xi=0}\ , \tag{6.7}$$

using Eq. (5.15).

The physical meaning of Eq. (6.2) is best understood by rewriting it in the form

$$\frac{1}{\bar{\rho}}\frac{dJ^a}{dt}+u^a(\partial^bu^b)=\frac{1}{m}F^a\ , \tag{6.8}$$

using the definition (5.28), and where the convective derivative d/dt is defined as usual by

$$\frac{d}{dt}\equiv\frac{\partial}{\partial t}+u^b\partial^b\ . \tag{6.9}$$

Finally, by combining Eq. (6.8) with the continuity equation (6.1), we arrive at Newton's equation of motion,

$$m\frac{d\mathbf{u}}{dt}=\mathbf{F}\ . \tag{6.10}$$

Just as for the current continuity equation, it is also again clear that the Newtonian equation of motion (6.10), or equivalently Eq. (6.2) for the momentum density, is true also at an arbitrary SUBn level of truncation. Even more important is the fact that these conservation laws are also valid when more drastic subapproximations are made which entail dropping extra terms from the evaluation of the expectation value $\bar{V}$ of the potential energy. Such subapproximations are often made in such realistic applications of the ECCM as to systems with hard-core interparticle forces. The reason for the continuing validity of the conservation laws even in these cases is that each term in $\bar{V}$ transforms in exactly the same way under the gauge transformation. That is, the symmetry is obeyed by each term separately.

Before proceeding to the second-order (in ξ^a) equation (5.27), we take this opportunity to emphasize the general nature of the above results, by making contact with the well-known f-sum rule. To this end, we specialize to the linearized regime close to the equilibrium point, and consider the effect of an external scalar field of an infinitesimal impulsive type,

$$\delta\phi(r,t)=\psi(r)\delta(t)\ . \tag{6.11}$$

From Eqs. (6.1)–(6.5) it is immediately apparent that the infinitesimal change in the number density $\delta\bar{\rho}(r,t)$ is continuous over the time $t=0$, but its time derivative changes discontinuously by an amount,

$$\delta\dot{\bar{\rho}}(r,0^+)=\frac{1}{m}\nabla\cdot[\bar{\rho}(r)\nabla\psi(r)]\ . \tag{6.12}$$

In terms of the density-density response function $\chi(r,r';t-t')$ defined as usual[19] with the aid of the Heisenberg picture operators, as

$$\begin{aligned}&\chi(r,r';t-t')\equiv 2i\theta(t-t')\chi''(r,r';t-t')\ ,\\&\chi''(r,r';t-t')\equiv\tfrac{1}{2}\langle[\rho(r,t),\rho(r',t')]\rangle\ ,\end{aligned} \tag{6.13}$$

the change in the number density can be expressed as

$$\delta\bar{\rho}(r,t)=-\int dr'\int dt'\chi(r,r';t-t')\delta\phi(r',t')\ , \tag{6.14}$$

where the minus sign in Eq. (6.14) is consistent with the sign convention for ϕ introduced in Eq. (3.6). In terms of Fourier transforms, defined as usual by

$$\chi''(r,r';t)\equiv\int_{-\infty}^{\infty}\frac{d\omega}{2\pi}e^{-i\omega t}\chi''(r,r';\omega)\ , \tag{6.15}$$

we trivially find the relation,

$$\dot{\chi}(r,r';t=0^+)=\frac{1}{\pi}\int_{-\infty}^{\infty}d\omega\,\omega\chi''(r,r';\omega)\ . \tag{6.16}$$

On the other hand, use of the Heisenberg equation of motion gives the relation

$$\dot{\chi}(r,r';t=0^+)=\langle[[\rho(r),H],\rho(r')]\rangle\ . \tag{6.17}$$

A straightforward evaluation of the double commutator in Eq. (6.17), and a comparison with Eq. (6.16), then leads immediately to the f-sum rule in the usual form,

$$\int_{-\infty}^{\infty}\frac{d\omega}{2\pi}\omega\chi''(r,r';\omega)=\frac{1}{2m}\nabla_r\cdot\nabla_{r'}[\bar{\rho}(r)\delta(r-r')]\ . \tag{6.18}$$

Returning to Eq. (6.14), and specializing to the impulsive perturbation of Eq. (6.11), it will be immediately obvious on the basis of Eqs. (6.16) and (6.18) that the result from the linear-response theory for $\delta\bar{\rho}(r,0^+)$ is precisely as given in Eq. (6.12) from our general formalism. In this spirit, the conservation law of Eq. (6.2) may be viewed as a natural generalization of the f-sum rule away from the linearized regime.

C. Equation of motion for the energy density

Finally, we turn our attention to the second-order (in ξ^a) equation (5.27), and reexpress it also in terms of the gauge-invariant quantities of Eqs. (5.18a)–(5.18c). Rather than express it directly as an equation of motion for the kinetic stress tensor, proportional to Γ^{ab}, it turns out to be more convenient to give the equation of motion for the tensor $K^{ab}(R)$, defined as,

$$K^{ab}(R)\equiv\tfrac{1}{2}m[\Gamma^{ab}(R)+\bar{\rho}(R)u^a(R)u^b(R)] , \tag{6.19}$$

which, as we shall see below, is related to the kinetic energy density. By making use of the previous equation of motion (6.2), we can show, after a straightforward but very laborious calculation, that K^{ab} obeys the equation of motion,

$$\begin{aligned}\frac{\partial K^{ab}}{\partial t}+\partial^c\Big[&\Delta^{abc}+u^aK^{bc}+u^bK^{ac}+u^cK^{ab}-m\bar{\rho}u^au^bu^c\\&+\frac{\bar{\rho}}{24m^2}(\epsilon^{bcd}\partial^aB^d+\epsilon^{acd}\partial^bB^d)\Big]\\=&\tfrac{1}{2}\bar{\rho}(W^{ab}+u^aE^b+u^bE^a)\\&+\frac{1}{m}(\epsilon^{bcd}K^{ac}+\epsilon^{acd}K^{bc})B^d ,\end{aligned} \tag{6.20}$$

where $\mathbf{E}$ and $\mathbf{B}$ are the "external force fields" defined in Eq. (6.5), and where ϵ^{abc} is the Levi-Civita symbol or antisymmetric unit tensor of third rank.

Just as Eq. (6.2) was used to study the conservation law of total momentum, we now show how Eq. (6.20) can be similarly used to study a comparable local form of the corresponding conservation law of total energy. In this way we may identify the energy current density and investigate possible local forms for the energy source density, particularly in the case that the external potentials are time dependent. The Hamiltonian of Eq. (3.6) breaks naturally into the sum $H=H_1+V$ of a one-body piece H_1 and the two-body piece V due to the pairwise interactions. The one-body piece leads to a contribution $\langle H_1\rangle\equiv\bar{H}_1$ to the energy-expectation value which may be written in terms of a local energy density functional $\epsilon_1(r)$ as

$$\begin{aligned}\bar{H}_1&=\int dr\,\epsilon_1(r) ,\\\epsilon_1(r)&=\left\langle\frac{1}{2m}(\nabla_ra_r^\dagger)\cdot(\nabla_ra_r)-\mathbf{j}(r)\cdot\mathbf{A}(r)\right.\\&\quad\left.+\rho(r)\left[\phi(r)-\mu+\frac{1}{2m}\mathbf{A}^2(r)\right]\right\rangle ,\end{aligned} \tag{6.21}$$

with $\rho(r)$ and $\mathbf{j}(r)$ the operators defined in Eq. (3.7). This expression is readily evaluated. In particular, by writing the first term in the form

$$\left\langle\frac{1}{2m}(\nabla_ra_r^\dagger)\cdot(\nabla_ra_r)\right\rangle=\frac{1}{2m}\lim_{r'\to r}\frac{\partial^2}{\partial r^a\partial r'^a}\bar{\rho}(r,r') , \tag{6.22}$$

and by employing Eqs. (5.10)–(5.12) and (5.18a), we find

$$\begin{aligned}\epsilon_1(R)=&\frac{1}{8m}\nabla_R^2\bar{\rho}(R)+\tfrac{1}{2}m\Gamma^{aa}(R)+\tfrac{1}{2}m\bar{\rho}(R)\mathbf{u}^2(R)\\&+\bar{\rho}(R)[\phi(R)-\mu] ,\end{aligned} \tag{6.23}$$

where $\mathbf{u}(R)$ is the gauge-invariant velocity field of Eq. (5.28). The third term, $\frac{1}{2}m\bar{\rho}\mathbf{u}^2$, in Eq. (6.23) is simply the hydrodynamical kinetic energy density of the average translational motion, whereas the second term $\frac{1}{2}m\,\mathrm{tr}(\Gamma)$, together with the first term, may be interpreted as the kinetic energy density in the local rest frame. Since the first term in Eq. (6.23) is a perfect divergence, its contribution to $\bar{H}_1$ vanishes, and hence it is, strictly speaking, redundant. However, its inclusion guarantees the positivity of the kinetic energy density. Other forms for the kinetic energy in the Hamiltonian of Eq. (3.6) which differ only by surface terms, but which do not guarantee this positivity, have also been considered.[20] We note that each of the terms in Eq. (6.23) is separately gauge invariant except for the potential energy term $\bar{\rho}\phi$ in the external field.

By comparison with the one-body energy, the two-body energy $\bar{V}$ of Eq. (4.11) cannot be simply expressed as the volume integral, $\bar{V}=\int dr\,\epsilon_2(r)$, of a local energy density functional $\epsilon_2(r)$. However, we show below that its time rate of change $\partial\bar{V}/\partial t$ does allow a convenient local expression. To this end we calculate the time derivative of the diagonal elements $D(r,r')$ of the two-particle density matrix, via the usual Heisenberg equation of motion,

$$\begin{aligned}\frac{\partial}{\partial t}\langle a_r^\dagger a_{r'}^\dagger a_{r'}a_r\rangle&=-i\langle[a_r^\dagger a_{r'}^\dagger a_{r'}a_r,H]\rangle\\&=-\nabla_r\cdot\langle a_{r'}^\dagger\mathbf{J}(r)a_{r'}\rangle-\nabla_{r'}\cdot\langle a_r^\dagger\mathbf{J}(r')a_r\rangle ,\end{aligned} \tag{6.24}$$

where we have used the Hamiltonian from Eq. (3.6), and have employed the definition (5.23) of the total current density operator $\mathbf{J}(r)$. Using Eqs. (4.10) and (4.11), we may thus write the time rate of change of the two-body energy as

$$\begin{aligned}\frac{\partial\bar{V}}{\partial t}&=\tfrac{1}{2}\int dr\int dr'v(r-r')\frac{\partial}{\partial t}\langle a_r^\dagger a_{r'}^\dagger a_{r'}a_r\rangle\\&=\frac{\partial}{\partial t}\int dr\,\epsilon_2(r) ,\end{aligned} \tag{6.25}$$

where from Eq. (6.24) we have defined $\epsilon_2(r)$ as

$$\frac{\partial\epsilon_2(r)}{\partial t}\equiv-\int dr'v(r-r')\nabla_r\cdot\langle a_{r'}^\dagger\mathbf{J}(r)a_{r'}\rangle . \tag{6.26}$$

By making use of the definition (5.22), it is trivial to show that Eq. (6.26) may be rewritten as

$$\frac{\partial \epsilon_2(r)}{\partial t} = -\tfrac{1}{2}\bar{\rho}(r) W^{aa}(r) - \nabla_r \cdot \mathbf{P}(r) , \tag{6.27}$$

with the local vector field $\mathbf{P}(r)$ defined as

$$\mathbf{P}(r) \equiv \int dr' v(r-r') \langle a_r^\dagger \mathbf{J}(r) a_{r'} \rangle . \tag{6.28}$$

It is clear that the field $\mathbf{P}(r)$ represents an energy flux due to the internal forces in which the interaction energy of any pair of particles one of which is at the space point r is associated in an asymmetric fashion wholly to the particle at the point r. Finally, we notice that by contrast with the one-body energy $\epsilon_1(r)$, Eq. (6.26) does not lead to any simple expression for $\epsilon_2(r)$ itself.

A combination of Eqs. (6.21) and (6.27) enables us to write a local form for the energy balance,

$$\frac{\partial \bar{H}}{\partial t} \equiv \int dr \frac{\partial \epsilon(r)}{\partial t} = \int dr \left[\frac{\partial \epsilon_1(r)}{\partial t} + \frac{\partial \epsilon_2(r)}{\partial t} \right] , \tag{6.29}$$

where the energy density $\epsilon(r)$ satisfies a continuity equation, which is readily found by employing our earlier result of Eqs. (6.19) and (6.20), together with Eq. (6.1). In this way, we find the energy-density continuity equation in the form

$$\frac{\partial \epsilon}{\partial t} + \nabla \cdot \mathbf{J}_\epsilon = S_\epsilon , \tag{6.30}$$

with the energy flux vector $\mathbf{J}_\epsilon$ given by

$$\mathbf{J}_\epsilon \equiv \mathbf{J}_\epsilon(r) \equiv \frac{1}{8m} \nabla^2 \mathbf{J} + \left[\frac{m}{2\bar{\rho}} \operatorname{tr}\Gamma + \tfrac{1}{2} m \mathbf{u}^2 + \phi - \mu \right] \mathbf{J} + (\Delta^{aab} + m u^a \Gamma^{ab}) \hat{\mathbf{r}}^b - \frac{\bar{\rho}}{12 m^2} \nabla \times \mathbf{B} + \mathbf{P} , \tag{6.31}$$

where $\hat{\mathbf{r}}^b$ is a unit vector in the b direction, and with the energy source density given by

$$S_\epsilon \equiv S_\epsilon(r) \equiv \bar{\rho} \frac{\partial \phi}{\partial t} - \mathbf{J} \cdot \frac{\partial \mathbf{A}}{\partial t} = \bar{\rho} \frac{d\phi}{dt} + \mathbf{J} \cdot \mathbf{E} , \tag{6.32}$$

where in the second form above we have employed the convective derivative of Eq. (6.9) and the external field $\mathbf{E}$ of Eq. (6.5).

Finally, we note that due to the presence of the terms involving the scalar field ϕ, none of the quantities $\epsilon(r)$, $\mathbf{J}_\epsilon(r)$ and $S_\epsilon(r)$ is gauge invariant. It is however, a trivial matter to rewrite Eq. (6.30) as a gauge-invariant balance equation of the form

$$\frac{\partial}{\partial t}(\epsilon - \phi\bar{\rho}) + \nabla \cdot (\mathbf{J}_\epsilon - \phi \mathbf{J}) = \mathbf{J} \cdot \mathbf{E} , \tag{6.33}$$

by combining it with the current continuity equation (6.1). We now see explicitly from Eqs. (6.23) and (6.31) that the subtracted energy density $(\epsilon - \phi\bar{\rho})$ and energy flux $(\mathbf{J}_\epsilon - \phi \mathbf{J})$ are gauge invariant, as is the source term $\mathbf{J} \cdot \mathbf{E}$ in Eq. (6.33).

VII. DISCUSSION

The earlier papers, I and II, of this series gave a comprehensive account of how the extended coupled-cluster amplitudes $\{\sigma_n, \bar{\sigma}_n\}$ can be used to parametrize the Hilbert space for an arbitrary many-body problem. A complete specification of the numerical values of these amplitudes corresponds to the specification of the representative point of the state of the system in the ECCM phase space. The phase space is a complex differentiable manifold with a symplectic structure induced by a classical Poisson bracket form. The equations of motion for the amplitudes $\{\sigma_n, \bar{\sigma}_n\}$ have the usual classical canonical form. The temporal behavior of the system is described by a trajectory in the phase space, along which the representative point moves. According to a modern view of statistical mechanics[21,22] it is the entire phase portrait, i.e., the totality of all trajectories, which is of interest to statistical physics and which leads to a proper qualitative description of the system. The more traditional approach to statistical mechanics at finite temperatures, $T > 0$, is based on the ensemble approach of Gibbs and the use of the statistical density operator. One might easily imagine the present ECCM approach being extended along similar lines by a more complete investigation of the geometrical properties of the ECCM phase space.

The present paper describes an application of the ECCM formalism to the case of a condensed Bose fluid. We have been mainly interested in the properties of a single trajectory instead of the whole phase portrait, and in this sense the present treatment forms only a modest beginning of a more comprehensive statistical theory. Nevertheless, we have been able to show that the individual trajectories in the ECCM phase space fully comply with the pertinent gauge symmetries and the local hydrodynamical conservation laws.

The hydrodynamically relevant variables are the local densities, such as the number density, current, and energy density. In forming the expressions for these quantities in terms of the phase-space coordinates $\{\sigma_n, \bar{\sigma}_n\}$ we have taken full advantage of the local $U(1)$ gauge symmetry following from the particle-number conservation. From the equations of motion for the amplitudes $\{\sigma_n, \bar{\sigma}_n\}$ we derived the balance equations for the particle-number density, current density, and energy density, and showed their connection to the cumulant expansion of the one-particle density matrix. All the hydrodynamical continuity equations so obtained are exact and expressed in a gauge-invariant form. The gauge invariance can be interpreted as the differential or local Galilean invariance. Hence our description is able, for example, to separate correctly the average translational (hydrodynamical) kinetic energy from the average kinetic energy in the local rest frame, a feature which has not usually been easy to carry through in a microscopic treatment (see, e.g., the discussion in Sec. 8 of Ref. 23).

As a technical remark it is worth mentioning that in order to get the continuity equations for the current and energy densities we have used the exact procedure and avoided making the conventional spatial smoothing approximation.[20,24] In the case of the energy density this is made possible by the fact that although the interparticle interaction energy cannot be expressed as a volume energy of any simple local density, its time derivative allows

such a local representation. Thus, even without the assumption of slow spatial variations, the time derivative of the energy density is given by a perfect divergence of the energy current, in addition to the local sources due to the external forces. On the other hand, the equation of motion for the particle-current density will be expressed in the conventional form in terms of a perfect divergence of the stress tensor only if the term arising from the interparticle interactions is subjected to the smoothing approximation.

The earlier-mentioned SUBn truncation schemes for the infinite hierarchy of the ECCM equations form a particular and natural set of approximations. It is an easy matter to show that all of the above continuity equations hold also in the SUBn approximations. As a matter of fact, the continuity equations will be satisfied by even more drastic approximations in which part of the terms contributing to the two-body density matrix are dropped away. This derives from the fact that each of the terms is separately fully gauge invariant. It was also shown that the correctness of the hydrodynamical equation of motion for the current density directly guarantees that the f-sum rule will be satisfied in the linearized regime. This, again, is true also for the SUBn truncations and the other approximations described above.

Baym and Kadanoff[25,26] have studied the conditions under which general diagram summations within the Green's-function formalism lead to the conservation of the hydrodynamical densities. Their result can be formulated in terms of a functional $\Phi[G]$ of the Green's function G by requiring the self-energy Σ to be given as the functional derivative of Φ with respect to G. A typical feature for such Φ-derivable approximations is that the perturbation series cannot be taken into account in such a way that all diagrams up to a certain power of interaction are included. Rather, the diagrams necessarily have to be rearranged differently in the summation, in a way where from each power only a chosen subset of diagrams is taken into account. This result is indeed qualitatively similar to our SUBn approximation schemes, which also have the property of extending to infinite order in the interaction, but summing only a subset in each order.

In conclusion, we emphasize again, however, that the ECCM approach has left its origins in perturbation theory far behind. We view the present paper as a first step towards the ultimate goal of expressing all physical observables and processes in terms of the geometrical properties of the underlying ECCM phase space. One of the next steps in this procedure will be the development of new approximation schemes based entirely on this geometrical approach, and which, conversely, go beyond such schemes as the SUBn scheme which still have some links with perturbation theory. The approach in I was based on a dynamic variational principle for the action and its potentially exact parametrization in terms of general ECCM states. Such time-evolution equations as our ECCM equations of motion for the basic amplitudes $\{\sigma_n,\tilde{\sigma}_n\}$, which have an underlying symplectic structure and which hence also have the possibility of being associated with suitably defined generalized Poisson brackets, have been discussed in other contexts by other authors. For example, a rather general account of the geometry of the time-dependent variational principle in quantum mechanics has been given by Kramer and Saraceno.[27] It may well be that further progress in our own geometrical approach to the ECCM will be made by exploring more deeply its connections to other such similar structures.

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APPENDIX A: EXPLICIT EXPRESSIONS FOR THE REDUCED SUBSYSTEM AMPLITUDES

In this appendix we evaluate the reduced subsystem amplitudes defined in Eqs. (4.9a) and (4.9b). The ϕ amplitudes are defined as

$$\phi_{n+2}(r,r';x_1,\ldots,x_n)\equiv\langle\Phi\mid\hat{a}_r^{\dagger}\hat{a}_{r'}^{\dagger}a_{x_1}^{\dagger}\cdots a_{x_n}^{\dagger}\mid\Phi\rangle\ . \tag{A1}$$

Using the definition of the doubly similarity-transformed operators from Eq. (2.8) and the definitions contained in Eqs. (2.11)–(2.14), we have

$$\hat{a}_r^{\dagger}=e^{\tilde{\Sigma}}a_r^{\dagger}e^{-\tilde{\Sigma}}=a_r^{\dagger}+[\tilde{\Sigma},a_r^{\dagger}]\ . \tag{A2}$$

Using Eq. (A2) in Eq. (A1), together with the relation $\langle\Phi\mid a_r^{\dagger}=0$, yields the relation

$$\phi_{n+2}(r,r';x_1,\ldots,x_n)=\langle\phi\mid\tilde{\Sigma}a_r^{\dagger}\{a_{r'}^{\dagger}+[\tilde{\Sigma},a_{r'}^{\dagger}]\}a_{x_1}^{\dagger}\cdots a_{x_n}^{\dagger}\mid\Phi\rangle\ . \tag{A3}$$

With the aid of Eqs. (2.13) and (2.14) and the basic commutation relations (2.9), Eq. (A3) may be immediately rewritten as

$$\begin{aligned}\phi_{n+2}(r,r';x_1,\ldots,x_n)&=\tilde{\sigma}_{n+2}(r,r',x_1,\ldots,x_n)\\&+\langle\Phi\mid\tilde{\Sigma}a_r^{\dagger}\sum_{m=1}^{\infty}\frac{1}{m!}\sum_{i=1}^{m}\int dy_1\cdots\int dy_m\,\tilde{\sigma}_m(y_1,\ldots,y_m)a_{y_1}\cdots a_{y_{i-1}}a_{y_{i+1}}\cdots a_{y_m}\delta(y_i-r')a_{x_1}^{\dagger}\cdots a_{x_n}^{\dagger}\mid\Phi\rangle\ .\end{aligned} \tag{A4}$$

Using the fact that the amplitude $\tilde{\sigma}_m(y_1,\ldots,y_m)$ is completely symmetric under permutations of its arguments, the

m terms in the i summation of Eq. (A4) are easily seen to be identical by suitably relabeling the dummy integration variables. Hence

$$\phi_{n+2}(r,r';x_1,\ldots,x_n)=\tilde{\sigma}_{n+2}(r,r',x_1,\ldots,x_n)+\sum_{m=1}^{\infty}\frac{1}{(m-1)!}\int dy_1\cdots\int dy_{m-1}\tilde{\sigma}_m(r',y_1,\ldots,y_{m-1})\times\langle\Phi\mid\tilde{\Sigma}a_r^{\dagger}Ia_{y_1}\cdots a_{y_{m-1}}a_{x_1}^{\dagger}\cdots a_{x_n}^{\dagger}\mid\Phi\rangle\ . \tag{A5}$$

Finally, inserting a resolution of the identity I of the form of Eq. (2.10) at the place so indicated in Eq. (A5), and relabeling the summation index $m=k+1$, we get

$$\phi_{n+2}(r,r';x_1,\ldots,x_n)=\tilde{\sigma}_{n+2}(r,r',x_1,\ldots,x_n)+\sum_{k=0}^{\infty}\frac{1}{k!}\sum_{l=0}^{\infty}\frac{1}{l!}\int dy_1\cdots\int dy_k\int dz_1\cdots\int dz_l\tilde{\sigma}_{k+1}(r',y_1,\ldots,y_k)\tilde{\sigma}_{l+1}(r,z_1,\ldots,z_l)\times\langle\Phi\mid a_{z_1}\cdots a_{z_l}a_{y_1}\cdots a_{y_k}a_{x_1}^{\dagger}\cdots a_{x_n}^{\dagger}\mid\Phi\rangle, \tag{A6}$$

where we have made use of Eq. (2.14) again. The trivial evaluation of the remaining matrix element in Eq. (A6) then gives the desired result,

$$\phi_{n+2}(r,r';x_1,\ldots,x_n)=\tilde{\sigma}_{n+2}(r,r',x_1,\ldots,x_n)+\sum_{l=0}^{n}\frac{1}{l!(n-l)!}\mathcal{S}_{(x_1,\ldots,x_n)}[\tilde{\sigma}_{l+1}(r,x_1,\ldots,x_l)\tilde{\sigma}_{n-l+1}(r',x_{l+1},\ldots,x_n)]\ , \tag{A7}$$

where the mode of action of the symmetrization operator $\mathcal{S}_{(x_1,\ldots,x_n)}$ is to sum over all $n!$ permutations of the arguments $x_1,\ldots,x_n$ of the function on which it operates. For example,

$$\mathcal{S}_{(x_1,x_2)}[f(x_1,x_2)]=f(x_1,x_2)+f(x_2,x_1)\ . \tag{A8}$$

We now turn our attention to the χ amplitudes, defined in Eq. (4.9b) as

$$\begin{aligned}\chi_{n+2}(r,r';x_1,\ldots,x_n)&\equiv\langle\Phi\mid a_{x_1}\cdots a_{x_n}\hat{a}_r\hat{a}_{r'}\mid\Phi\rangle\\&=\langle\Phi\mid a_{x_1}\cdots a_{x_n}e^{S''}e^{-S}a_ra_{r'}e^{S}e^{-S''}\mid\Phi\rangle\\&=\langle\Phi\mid e^{S''}a_{x_1}\cdots a_{x_n}e^{-S}a_re^{-S}e^{S}a_{r'}e^{S}\mid\Phi\rangle\ ,\end{aligned} \tag{A9}$$

where we have used Eq. (2.11) and the fact that $a_x\mid\Phi\rangle=0$. We may now use the relation

$$e^{-S}a_re^{S}=a_r+[a_r,S]\ , \tag{A10}$$

and the equivalent relation for $a_{r'}$, together with the relation $a_{r'}\mid\Phi\rangle=0$, to write Eq. (A10) as

$$\begin{aligned}\chi_{n+2}(r,r';x_1,\ldots,x_n)&=\langle\Phi\mid e^{S''}a_{x_1}\cdots a_{x_n}\{a_r+[a_r,S]\}a_{r'}S\mid\Phi\rangle\\&=\sigma_{n+2}(r,r',x_1,\ldots,x_n)+\langle\Phi\mid e^{S''}a_{x_1}\cdots a_{x_n}[a_r,S]e^{-S''}Ie^{S''}a_{r'}S\mid\Phi\rangle\ ,\end{aligned} \tag{A11}$$

where we have used the definition (2.14), and have inserted a unit operator of the form $(e^{-S''}Ie^{S''})$ in the last term, as shown. If we now insert a resolution of this last identity I of the form of Eq. (2.10), we have

$$\chi_{n+2}(r,r';x_1,\ldots,x_n)=\sigma_{n+2}(r,r',x_1,\ldots,x_n)+\sum_{l=0}^{\infty}\frac{1}{l!}\int dz_1\cdots\int dz_l\langle\Phi\mid e^{S''}a_{x_1}\cdots a_{x_n}[a_r,S]e^{-S''}a_{z_1}^{\dagger}\cdots a_{z_l}^{\dagger}\mid\Phi\rangle\times\langle\Phi\mid a_{z_1}\cdots a_{z_l}a_{r'}e^{S''}S\mid\Phi\rangle\ . \tag{A12}$$

The $l=0$ term in the above summation may now profitably be split off the remainder of the sum. Equation (A12) may then be written, using $e^{-S''}\mid\Phi\rangle=\mid\Phi\rangle$ and $a_r\mid\Phi\rangle=0$, as

$$\chi_{n+2}(r,r';x_1,\ldots,x_n)=\sigma_{n+2}(r,r',x_1,\ldots,x_n)+\sigma_{n+1}(r,x_1,\ldots,x_n)\sigma_1(r')$$
$$+\sum_{l=1}^{\infty}\frac{1}{l!}\int dz_1\cdots\int dz_l\langle\Phi\,|\,e^{S''}a_{x_1}\cdots a_{x_n}[a_r,S]Ie^{-S''}a^{\dagger}_{z_1}\cdots a^{\dagger}_{z_l}\,|\,\Phi\rangle\sigma_{l+1}(r',z_1,\ldots,z_l)\,, \tag{A13}$$

where we have used Eq. (2.14). We now insert again a resolution of the identity of the form of Eq. (2.10) in the place indicated by the unit operator I in Eq. (A13). Hence,

$$\chi_{n+2}(r,r';x_1,\ldots,x_n)$$
$$=\sigma_{n+2}(r,r',x_1,\ldots,x_n)+\sigma_{n+1}(r,x_1,\ldots,x_n)\sigma_1(r')$$
$$+\sum_{l=1}^{\infty}\frac{1}{l!}\int dz_1\cdots\int dz_l\sum_{j=0}^{\infty}\frac{1}{j!}\int du_1\cdots\int du_j\langle\Phi\,|\,e^{S''}a_{x_1}\cdots a_{x_n}[a_r,S]a^{\dagger}_{u_1}\cdots a^{\dagger}_{u_j}\,|\,\Phi\rangle$$
$$\times\langle\Phi\,|\,a_{u_1}\cdots a_{u_j}e^{-S''}a^{\dagger}_{z_1}\cdots a^{\dagger}_{z_l}\,|\,\Phi\rangle\sigma_{l+1}(r',z_1,\ldots,z_l)\,. \tag{A14}$$

From Eq. (2.11) it is clear that the commutator $[a_r,S]$ in Eq. (A14) is composed of no destruction operators, and hence may be commuted through the product $a^{\dagger}_{u_1}\cdots a^{\dagger}_{u_j}$. We may then use the relation $a_r\,|\,\Phi\rangle=0$ again to write Eq. (A14) as

$$\chi_{n+2}(r,r';x_1,\ldots,x_n)$$
$$=\sigma_{n+2}(r,r',x_1,\ldots,x_n)+\sigma_{n+1}(r,x_1,\ldots,x_n)\sigma_1(r')$$
$$+\sum_{l=1}^{\infty}\frac{1}{l!}\sum_{j=0}^{\infty}\frac{1}{j!}\int dz_1\cdots\int dz_l\int du_1\cdots\int du_j\langle\Phi\,|\,e^{S''}a_{x_1}\cdots a_{x_n}a^{\dagger}_{u_1}\cdots a^{\dagger}_{u_j}e^{-S''}Ie^{S''}a_rS\,|\,\Phi\rangle$$
$$\times\langle\Phi\,|\,a_{u_1}\cdots a_{u_j}e^{-S''}a^{\dagger}_{z_1}\cdots a^{\dagger}_{z_l}\,|\,\Phi\rangle\sigma_{l+1}(r',z_1,\ldots,z_l)\,, \tag{A15}$$

wherein we have inserted the identity factor $e^{-S''}Ie^{S''}$ as shown in the first matrix element of the last term. A further resolution of this identity I of the form of Eq. (2.10) then gives

$$\chi_{n+2}(r,r';x_1,\ldots,x_n)$$
$$=\sigma_{n+2}(r,r',x_1,\ldots,x_n)+\sigma_{n+1}(r,x_1,\ldots,x_n)\sigma_1(r')$$
$$+\sum_{l=1}^{\infty}\frac{1}{l!}\sum_{j=0}^{\infty}\frac{1}{j!}\sum_{k=0}^{\infty}\frac{1}{k!}\int dz_1\cdots\int dz_l\int du_1\cdots\int du_j\int dy_1\cdots\int dy_k\sigma_{l+1}(r',z_1,\ldots,z_l)$$
$$\times\langle\Phi\,|\,e^{S''}a_{x_1}\cdots a_{x_n}a^{\dagger}_{u_1}\cdots a^{\dagger}_{u_j}e^{-S''}a^{\dagger}_{y_1}\cdots a^{\dagger}_{y_k}\,|\,\Phi\rangle$$
$$\times\langle\Phi\,|\,a_{y_1}\cdots a_{y_k}e^{S''}a_rS\,|\,\Phi\rangle$$
$$\times\langle\Phi\,|\,a_{u_1}\cdots a_{u_j}e^{-S''}a^{\dagger}_{z_1}\cdots a^{\dagger}_{z_l}\,|\,\Phi\rangle\,. \tag{A16}$$

The $k=0$ term in the k summation of Eq. (A16) may now, again, profitably be separated from the remainder of the sum. Using $e^{-S''}\,|\,\Phi\rangle=\,|\,\Phi\rangle$, the j summation may be reperformed in this $k=0$ term, to give

$$\chi_{n+2}(r,r';x_1,\ldots,x_n)$$
$$=\sigma_{n+2}(r,r',x_1,\ldots,x_n)+\sigma_{n+1}(r,x_1,\ldots,x_n)\sigma_1(r')$$
$$+\sum_{l=1}^{\infty}\frac{1}{l!}\int dz_1\cdots\int dz_l\sigma_{l+1}(r',z_1,\ldots,z_l)\langle\Phi\,|\,e^{S''}a_{x_1}\cdots a_{x_n}e^{-S''}a^{\dagger}_{z_1}\cdots a^{\dagger}_{z_l}\,|\,\Phi\rangle\sigma_1(r)$$
$$+\sum_{k=1}^{\infty}\frac{1}{k!}\sum_{l=1}^{\infty}\frac{1}{l!}\int dy_1\cdots\int dy_k\int dz_1\cdots\int dz_l\sigma_{k+1}(r,y_1,\ldots,y_k)\sigma_{l+1}(r',z_1,\ldots,z_l)$$
$$\times\sum_{j=0}^{\infty}\frac{1}{j!}\int du_1\cdots\int du_j\langle\Phi\,|\,e^{S''}a_{x_1}\cdots a_{x_n}a^{\dagger}_{u_1}\cdots a^{\dagger}_{u_j}Ie^{-S''}a^{\dagger}_{y_1}\cdots a^{\dagger}_{y_k}\,|\,\Phi\rangle$$
$$\times\langle\Phi\,|\,a_{u_1}\cdots a_{u_j}e^{-S''}a^{\dagger}_{z_1}\cdots a^{\dagger}_{z_l}\,|\,\Phi\rangle\,, \tag{A17}$$

where we have used the definition (2.14) again. In conclusion, insertion of a last resolution of the identity of the form of Eq. (2.10) in the place marked I in Eq. (A17) leads to the final result

$$\chi_{n+2}(r,r';x_1,\ldots,x_n)=\sigma_{n+2}(r,r',x_1,\ldots,x_n)+\sigma_{n+1}(r,x_1,\ldots,x_n)\sigma_1(r')+\sigma_1(r)\sigma_{n+1}(r',x_1,\ldots,x_n)(1-\delta_{n0})$$
$$+\sum_{k=1}^{\infty}\frac{1}{k!}\sum_{l=1}^{\infty}\frac{1}{l!}\int dy_1\cdots\int dy_k\int dz_1\cdots\int dz_l\sigma_{k+1}(r,y_1,\ldots,y_k)\sigma_{l+1}(r',z_1,\ldots,z_l)$$
$$\times L_{kl}^n(x_1,\ldots,x_n\,|\,y_1,\ldots,y_k;z_1,\ldots,z_l)\,, \tag{A18}$$

where the coefficient L_{kl}^n is defined as

$$L_{kl}^n(x_1,\ldots,x_n\,|\,y_1,\ldots,y_k;z_1,\ldots,z_l)$$
$$\equiv\sum_{j=0}^{\infty}\frac{1}{j!}\sum_{m=0}^{\infty}\frac{1}{m!}\int du_1\cdots\int du_j\int dv_1\cdots\int dv_m\langle\Phi\,|\,e^{S''}a_{x_1}\cdots a_{x_n}a_{u_1}^{\dagger}\cdots a_{u_j}^{\dagger}a_{v_1}^{\dagger}\cdots a_{v_m}^{\dagger}\,|\,\Phi\rangle$$
$$\times\langle\Phi\,|\,e^{-S''}a_{u_1}\cdots a_{u_j}a_{z_1}^{\dagger}\cdots a_{z_l}^{\dagger}\,|\,\Phi\rangle\langle\Phi\,|\,e^{-S''}a_{v_1}\cdots a_{v_m}a_{y_1}^{\dagger}\cdots a_{y_k}^{\dagger}\,|\,\Phi\rangle\,, \tag{A19}$$

and is precisely the same coefficient as defined in I, written now in the real-space coordinate representation employed here.

APPENDIX B: ALTERNATIVE FORM OF THE TWO-BODY DENSITY MATRIX

The two-body density matrix $\langle a_{r_1}^{\dagger}a_{r_2}^{\dagger}a_{r_3}a_{r_4}\rangle$ is given in Eq. (4.8) in terms of the reduced subsystem amplitudes ϕ and χ, which are evaluated in detail in Appendix A. Here we present an alternative decomposition of $\langle a_{r_1}^{\dagger}a_{r_2}^{\dagger}a_{r_3}a_{r_4}\rangle$ with the aid of functional derivatives of the one-body density matrices $\langle a_r^{\dagger}a_{r'}\rangle$. We begin by writing

$$\langle a_{r_1}^{\dagger}a_{r_2}^{\dagger}a_{r_3}a_{r_4}\rangle=\langle\Phi\,|\,\hat{a}_{r_1}^{\dagger}\hat{a}_{r_4}\hat{a}_{r_2}^{\dagger}\hat{a}_{r_3}\,|\,\Phi\rangle-\langle\Phi\,|\,\hat{a}_{r_1}^{\dagger}\hat{a}_{r_3}\,|\,\Phi\rangle\delta(r_2-r_4)$$
$$=\langle\rho(r_1,r_4)\rho(r_2,r_3)\rangle-\bar{\rho}(r_1,r_3)\delta(r_2-r_4)\,, \tag{B1}$$

where we have used the definitions in Eqs. (4.7), (4.1), and (4.2). The general functional derivative techniques of I can now be applied to evaluate the first term on the right-hand side of Eq. (B1). To this effect, we first insert the resolution of the identity of the form of Eq. (2.10) between the two operators ρ, which then yields the relation

$$\langle\rho(r_1,r_4)\rho(r_2,r_3)\rangle=\bar{\rho}(r_1,r_4)\bar{\rho}(r_2,r_3)$$
$$+\sum_{n=1}^{\infty}\frac{1}{n!}\int dx_1\cdots\int dx_n\langle\Phi\,|\,\hat{\rho}(r_1,r_4)a_{x_1}^{\dagger}\cdots a_{x_n}^{\dagger}\,|\,\Phi\rangle\langle\Phi\,|\,a_{x_n}\cdots a_{x_1}\hat{\rho}(r_2,r_3)\,|\,\Phi\rangle\,, \tag{B2}$$

where the $n=0$ term of Eq. (2.10) has been split off to produce the term $\bar{\rho}(r_1,r_4)\bar{\rho}(r_2,r_3)$.

The two matrix elements in the remaining sum in Eq. (B2) can conveniently be expressed as functional derivatives of the respective one-body operator averages $\bar{\rho}(r_1,r_4)$ and $\bar{\rho}(r_2,r_3)$ with respect to the ECCM amplitudes $\{\sigma_n,\tilde{\sigma}_n\}$. This was shown in detail in I for the case of the product of two arbitrary operators. Following that treatment, we can write for the second matrix element in Eq. (B2)

$$\langle\Phi\,|\,a_{x_n}\cdots a_{x_1}\hat{\rho}(r_2,r_3)\,|\,\Phi\rangle=\langle\Phi\,|\,a_{x_n}\cdots a_{x_1}e^{S''}e^{-S}a_{r_2}^{\dagger}a_{r_3}e^{S}\,|\,\Phi\rangle$$
$$=\frac{\delta}{\delta S_n''(x_1,\ldots,x_n)}\langle\Phi\,|\,e^{S''}e^{-S}a_{r_2}^{\dagger}a_{r_3}e^{S}\,|\,\Phi\rangle\,|_S$$
$$=\left.\frac{\delta\bar{\rho}(r_2,r_3)}{\delta S_n''(x_1,\ldots,x_n)}\right|_S. \tag{B3}$$

As was pointed out earlier in the main text, it is more convenient to formulate the ECCM theory in terms of the amplitudes $\{\sigma_n,\tilde{\sigma}_n\}$, and thus we express the functional derivative in Eq. (B3) as

$$\left.\frac{\delta\bar{\rho}(r_2,r_3)}{\delta S_n''(x_1,\ldots,x_n)}\right|_S$$

$$=\sum_{m=1}^{\infty}\frac{1}{m!}\int dy_1\cdots\int dy_m\left[\frac{\delta\tilde{\sigma}_m(y_1,\ldots,y_m)}{\delta S_n''(x_1,\ldots,x_n)}\frac{\delta\bar{\rho}(r_2,r_3)}{\delta\tilde{\sigma}_m(y_1,\ldots,y_m)}+\frac{\delta\sigma_m(y_1,\ldots,y_m)}{\delta S_n''(x_1,\ldots,x_n)}\frac{\delta\bar{\rho}(r_2,r_3)}{\delta\sigma_m(y_1,\ldots,y_m)}\right]$$

$$=\frac{\delta\bar{\rho}(r_2,r_3)}{\delta\tilde{\sigma}_n(x_1,\ldots,x_n)}+\sum_{m=1}^{\infty}\frac{1}{m!}\int dy_1\cdots\int dy_m\sigma_{n+m}(x_1,\ldots,x_n,y_1,\ldots,y_m)\frac{\delta\bar{\rho}(r_2,r_3)}{\delta\sigma_m(y_1,\ldots,y_m)}\ . \tag{B4}$$

Here we have employed Eqs. (2.13) and (2.14), which give the amplitudes σ_n and $\tilde{\sigma}_n$ as functionals of S'' and S and the fact that all the amplitudes are completely symmetric under permutation of their arguments.

Likewise we can transform the other matrix element in Eq. (B2) into an expression containing functional derivatives of $\bar{\rho}(r_1,r_4)$ with respect to σ_n and $\tilde{\sigma}_n$. In this case we will need, in addition to the functional derivatives with respect to $S_n''(x_1,\ldots,x_n)$ in Eq. (B4), also the derivatives with respect to $S_n(x_1,\ldots,x_n)$, which are defined analogously to Eq. (B4) to be

$$\left.\frac{\delta\bar{\rho}(r_1,r_4)}{\delta S_n(x_1,\ldots,x_n)}\right|_{S''}$$

$$=\sum_{m=1}^{\infty}\frac{1}{m!}\int dy_1\cdots\int dy_m\left[\frac{\delta\bar{\rho}(r_1,r_4)}{\delta\sigma_m(y_1,\ldots,y_m)}\frac{\delta\sigma_m(y_1,\ldots,y_m)}{\delta S_n(x_1,\ldots,x_n)}+\frac{\delta\bar{\rho}(r_1,r_4)}{\delta\tilde{\sigma}_m(y_1,\ldots,y_m)}\frac{\delta\tilde{\sigma}_m(y_1,\ldots,y_m)}{\delta S_n(x_1,\ldots,x_n)}\right]$$

$$=\sum_{m=1}^{\infty}\frac{1}{m!}\int dy_1\cdots\int dy_m\frac{\delta\bar{\rho}(r_1,r_4)}{\delta\sigma_m(y_1,\ldots,y_m)}$$

$$\times\left\langle\Phi\mid a_{y_m}\cdots a_{y_1}e^{S''}\sum_{k=1}^{\infty}\frac{1}{k!}\int dz_1\cdots\int dz_k\frac{\delta S_k(z_1,\ldots,z_k)}{\delta S_n(x_1,\ldots,x_n)}a_{z_1}^{\dagger}\cdots a_{z_k}^{\dagger}\mid\Phi\right\rangle$$

$$=\sum_{m=1}^{\infty}\frac{1}{m!}\int dy_1\cdots\int dy_m\frac{\delta\bar{\rho}(r_1,r_4)}{\delta\sigma_m(y_1,\ldots,y_m)}\langle\Phi\mid e^{S''}a_{y_m}\cdots a_{y_1}a_{x_1}^{\dagger}\cdots a_{x_n}^{\dagger}\mid\Phi\rangle\ . \tag{B5}$$

Here we have used the definitions in Eqs. (2.11) and (2.14). The matrix element on the last line of Eq. (B5) is a functional of the amplitudes $\tilde{\sigma}_n$ [cf. Eq. (3.22) of I]. Having now obtained the functional derivatives with respect to $S_n''(x_1,\ldots,x_n)$ and $S_n(x_1,\ldots,x_n)$, the remaining matrix element in Eq. (B2) can be calculated by applying methods similar to those used in Appendix A. We omit the rather lengthy calculation, and give only the resulting final expression (see I for details),

$$\langle\Phi\mid\hat{\rho}(r_1,r_4)a_{x_1}^{\dagger}\cdots a_{x_n}^{\dagger}\mid\Phi\rangle$$

$$=\frac{\delta\bar{\rho}(r_1,r_4)}{\delta\sigma_n(x_1,\ldots,x_n)}+\sum_{m=1}^{\infty}\frac{1}{m!}\int dy_1\cdots\int dy_m\frac{\delta\bar{\rho}(r_1,r_4)}{\delta\tilde{\sigma}_m(y_1,\ldots,y_m)}L_{mn}(y_1,\ldots,y_m;x_1,\ldots,x_n)$$

$$+\sum_{m=1}^{\infty}\frac{1}{m!}\sum_{k=1}^{\infty}\frac{1}{k!}\int dy_1\cdots\int dy_m\int dz_1\cdots\int dz_k\frac{\delta\bar{\rho}(r_1,r_4)}{\delta\sigma_m(y_1,\ldots,y_m)}\sigma_{m+k}(y_1,\ldots,y_m,z_1,\ldots,z_k)$$

$$\times L_{kn}(z_1,\ldots,z_k;x_1,\ldots,x_n)\ . \tag{B6}$$

Here the coefficient L_{kl} is defined as

$$L_{kl}(y_1,\ldots,y_k;z_1,\ldots,z_l)\equiv L_{lk}(z_1,\ldots,z_l;y_1,\ldots,y_k)$$

$$=\sum_{m=0}^{\infty}\frac{1}{m!}\sum_{n=0}^{\infty}\frac{1}{n!}\int du_1\cdots\int du_m\int dv_1\cdots\int dv_n\langle\Phi\mid e^{S''}a_{u_1}^{\dagger}\cdots a_{u_m}^{\dagger}a_{v_1}^{\dagger}\cdots a_{v_n}^{\dagger}\mid\Phi\rangle$$

$$\times\langle\Phi\mid e^{-S''}a_{u_1}\cdots a_{u_m}a_{z_1}^{\dagger}\cdots a_{z_l}^{\dagger}\mid\Phi\rangle\langle\Phi\mid e^{-S''}a_{v_1}\cdots a_{v_n}a_{y_1}^{\dagger}\cdots a_{y_k}^{\dagger}\mid\Phi\rangle\ . \tag{B7}$$

We note that the coefficient L_{kl} is simply the special case L_{kl}^0 of Eq. (A19).

When we insert Eqs. (B3) and (B6) in Eq. (B2) and execute the implied multiplication, we obtain $\langle\rho(r_1,r_4)\rho(r_2,r_3)\rangle$ in terms of various products of the functional derivatives $\delta\bar{\rho}/\delta\sigma_n$ and $\delta\bar{\rho}/\delta\tilde{\sigma}_n$, multiplied with coefficients that them-

selves are functionals of σ_n and $\tilde{\sigma}_n$. These functional derivatives $\delta\bar{\rho}/\delta\sigma_n$ and $\delta\bar{\rho}/\delta\tilde{\sigma}_n$ are simple expressions of $\tilde{\sigma}_n$ and σ_n, respectively, as can be seen from Eq. (4.18). Furthermore, we notice that the last term in Eq. (B1), $-\bar{\rho}(r_1,r_3)\delta(r_2-r_4)$, will be canceled against a part of the product of terms $\delta\bar{\rho}(r_1,r_4)/\delta\sigma_n(x_1,\ldots,x_n)$ in Eq. (B6) and $\delta\bar{\rho}(r_2,r_3)/\delta\tilde{\sigma}_n(x_1,\ldots,x_n)$ in Eq. (B4). This is evident by inspecting Eq. (4.18). Omitting further details, we obtain the final expression

$$\begin{aligned}\langle a_{r_1}^\dagger a_{r_2}^\dagger a_{r_3} a_{r_4}\rangle &= \bar{\rho}(r_1,r_4)\bar{\rho}(r_2,r_3)+\sum_{n=0}^{\infty}\frac{1}{n!}\int dx_1\cdots\int dx_n\,\tilde{\sigma}_{n+2}(r_1,r_2,x_1,\ldots,x_n)\sigma_{n+2}(r_3,r_4,x_1,\ldots,x_n)\\
&+\sum_{n=0}^{\infty}\frac{1}{n!}\sum_{m=0}^{\infty}\frac{1}{m!}\int dx_1\cdots\int dx_n\int dy_1\cdots\int dy_m\\
&\times[\,\tilde{\sigma}_{n+1}(r_1,x_1,\ldots,x_n)Y^{11}_{n+1,m+1}(r_4,x_1,\ldots,x_n;r_3,y_1,\ldots,y_m)\tilde{\sigma}_{m+1}(r_2,y_1,\ldots,y_m)\\
&+\tilde{\sigma}_{n+1}(r_1,x_1,\ldots,x_n)Y^{12}_{n+1,m+1}(r_4,x_1,\ldots,x_n;r_2,y_1,\ldots,y_m)\sigma_{m+1}(r_3,y_1,\ldots,y_m)\\
&+\sigma_{n+1}(r_4,x_1,\ldots,x_n)Y^{21}_{n+1,m+1}(r_1,x_1,\ldots,x_n;r_3,y_1,\ldots,y_m)\tilde{\sigma}_{m+1}(r_2,y_1,\ldots,y_m)\\
&+\sigma_{n+1}(r_4,x_1,\ldots,x_n)Y^{22}_{n+1,m+1}(r_1,x_1,\ldots,x_n;r_2,y_1,\ldots,y_m)\sigma_{m+1}(r_3,y_1,\ldots,y_m)\,]\,. \qquad \text{(B8)}\end{aligned}$$

The various Y coefficients are functionals of the amplitudes σ_n and $\tilde{\sigma}_n$, with the following explicit forms:

$$\begin{aligned}&Y^{11}_{nm}(x_1,\ldots,x_n;y_1,\ldots,y_m)\\
&\quad=Y^{11}_{mn}(y_1,\ldots,y_m;x_1,\ldots,x_n)\equiv\sigma_{n+m}(x_1,\ldots,x_n,y_1,\ldots,y_m)\\
&\qquad+\sum_{k=1}^{\infty}\frac{1}{k!}\sum_{l=1}^{\infty}\frac{1}{l!}\int dz_1\cdots\int dz_k\int dv_1\cdots\int dv_l\,\sigma_{n+k}(x_1,\ldots,x_n,z_1,\ldots,z_k)\\
&\qquad\qquad\times L_{kl}(z_1,\ldots,z_k;v_1,\ldots,v_l)\sigma_{l+m}(v_1,\ldots,v_l,y_1,\ldots,y_m)\,,\\
&Y^{12}_{nm}(x_1,\ldots,x_n;y_1,\ldots,y_m)\equiv\sum_{k=1}^{\infty}\frac{1}{k!}\int dz_1\cdots\int dz_k\,\sigma_{n+k}(x_1,\ldots,x_n,z_1,\ldots,z_k)L_{km}(z_1,\ldots,z_k;y_1,\ldots,y_m)\,,\\
&Y^{21}_{nm}(x_1,\ldots,x_n;y_1,\ldots,y_m)\equiv Y^{12}_{mn}(y_1,\ldots,y_m;x_1,\ldots,x_n)\,, \qquad \text{(B9)}\\
&Y^{22}_{nm}(x_1,\ldots,x_n;y_1,\ldots,y_m)\equiv L_{nm}(x_1,\ldots,x_n;y_1,\ldots,y_m)\,.\end{aligned}$$

We point out that the expression of Eq. (B8) is trivially seen to be manifestly symmetric under the simultaneous interchange of the arguments $r_1\rightleftarrows r_2$ and $r_3\rightleftarrows r_4$, by making the appropriate change of integration variables and by using the symmetry relations between the Y coefficients as in the defining relations (B9). However, the symmetry under the interchange of either $r_1\rightleftarrows r_2$ or $r_3\rightleftarrows r_4$ separately is not manifest, since the first term on the right-hand side already does not show this symmetry. Indeed, to restore the symmetry it is clear that the remaining terms must contain some suitably disconnected pieces. We would only point out now that the structure of the L_{mn} coefficients is such that they are not completely connected, and that it is the contribution from the Y^{22} term in Eq. (B8) that properly accounts for this feature. The dedicated reader may prove to his satisfaction that once one has removed from this term the disconnected pieces [which are $\bar{\rho}(r_1,r_3)\bar{\rho}(r_2,r_4)$ and a part contributing to $\langle a_{r_1}^\dagger a_{r_2}^\dagger\rangle\langle a_{r_3}a_{r_4}\rangle$, where the remaining contribution to the latter product comes from the $n=0$ part of the second term in Eq. (B8)], all of the remaining terms are manifestly symmetric and connected, and that the total expression of Eq. (B8) does indeed obey all the correct symmetry properties.

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