Independent-Cluster Parametrizations of Wave Functions in Model Field Theories. II. Classical Mappings and Their Algebraic Structure

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Independent-cluster methods (ICM) are, on the one hand, perturbative, diagrammatically formulated, field-theoretic approaches to the quantum many-body problem. Nevertheless, at the same time they are variational and nonperturbative and permit a complete study of the dynamics of the pure quantal state. The methods divide into three principal classes, namely the configuration-interaction method, the normal coupled cluster method, and the extended coupled cluster method, which differ from each other mainly in the degree to which the basic amplitudes which parametrize the quantum mechanical state are connected. Each of the methods introduces a particular differentiable ICM manifold which is endowed with a symplectic structure. The basic ICM amplitudes provide the local coordinates on these manifolds. In this paper we are concerned with the algebraic structure of these methods and derive a number of rigorous mathematical results, using the anharmonic oscillator with its infinite-dimensional Hilbert space as a nontrivial example. The principal tool in this analysis is the Bargmann Hilbert space representation, which maps the operator algebra in the bosonic Hilbert space into the algebra of differential operators acting on functions of a complex variable. We study in detail the "ICM star product" which is a newly introduced algebraic structure on the ICM manifolds. It provides a classical map for the operator algebra, and can, for example, be used to map the quantum mechanical commutator into the classical Poisson bracket. Comparisons are also made with the Moyal star product and the more general deformation theory, which provide an autonomous route to quantization, namely the "star product quantization." They are naturally related to such topical theories as quantum groups. We also point out that the present methods allow a purely algebraic approach to deal with diagrammatic expansions, and we consider the structure of the various ICM diagrams from this algebraic point of view. © 1993 Academic Press, Inc.

I. INTRODUCTION

Coupled cluster (CC) theory is an *ab initio*, fully microscopic formulation of quantum many-body theory, which has been widely applied to a broad spectrum of many-body systems of interest in physics and chemistry. The coupled cluster method (CCM), or $\exp(S)$ method as it was then called, was first introduced by Coester [1] and further developed both by Kümmel and his co-workers [2–5] and by the quantum chemists [6–8]. Broad overviews which outline the method and indicate the diversity of its applications and their considerable degree of numerical success for both finite systems (e.g., atoms, molecules, nuclei) and infinite systems (e.g., nuclear matter, electron gas, quantum anti-ferromagnets), have been given recently in Refs. [9–11].

Understandably, in the past the major effort in CC theory has been expended on developing powerful approximation schemes which have wide applicability, are capable of systematic improvement, and yield results of very high accuracy at attainable levels of implementation. The very success in fulfilling these goals has, however, somewhat eclipsed the parallel development of a deeper analysis of the mathematical underpinnings of the method. One of our main aims in the first work in the present series [12] (hereafter referred to as I) was to redress this imbalance. A particular motivation was to continue the study of such fundamental foundations of the CCM as its existence and convergence properties. This had been initiated in an investigation by the present authors [13] of a holomorphic representation approach to the regularization of model field theories parametrized via CC techniques.

Coupled cluster theory exists in two main versions, namely the normal coupled cluster method (NCCM) and the extended coupled cluster method (ECCM) [14]. We showed in I how the configuration-interaction method (CIM) [15], or generalized shell model, forms a rather natural closed triad of formulations of quantum many-body theory, together with the NCCM and ECCM. We refer to them generically as independent-cluster (IC) methods. The primary, but fundamental, difference between them is the degree to which they incorporate at various levels of approximate implementation the exact size-extensivity or size-consistency features [16–19]. In the usual diagrammatic language (of Goldstone perturbation theory, for example), such considerations manifest themselves via the connectivity or linkedness properties of the associated diagrams for the subsystem amplitudes [14] that formally provide a complete set of parameters for each IC method (ICM). In turn, such extensivity and separability properties are intimately connected with the locality (or, more specifically, the quasilocality or multilocality) properties of the multiconfigurational IC subsystem amplitudes themselves.

We showed in detail in I, and recapitulate here in Section II, how the temporal evolution of the multiconfigurational amplitudes $\{x_I, \tilde{x}_I\}$ that characterize each ICM is described by classical canonical equations of motion in terms of some well-specified classical Hamiltonian functional, $\bar{H}[x_I, \tilde{x}_I]$, in each case. Each ICM may

also be regarded as performing a definite "bosonization" [20] and, in general, also "fermionization" [21] of the original Hilbert space $\mathcal{H}$ onto the subset of coherent states in a larger bosonized and fermionized space $\mathcal{B}^*$ in which $\mathcal{H}$ is imbedded. The ideal bosons and fermions in $\mathcal{B}^*$ carry the same multiconfigurational index labels $\{I\}$ as the IC subsystem amplitudes, and there is a one-to-one correspondence between them in each case.

Each IC classical Hamiltonian functional $\bar{H}[x_I, \tilde{x}_I]$ is defined in some classical phase space Γ_{phys}^H , which is itself a submanifold of the space Γ^H spanned by all points $(x_I, \tilde{x}_I)$. We have emphasized in I how the states generated by each ICM may be viewed as a well-defined set of *supercoherent states* in $\mathcal{H}$ associated with each point $(x_I, \tilde{x}_I)$ in Γ^H . While the usual coherent states in $\mathcal{H}$ (e.g., the one-particle Glauber or the two-particle "squeezed" coherent states) are typically used to introduce a *quasiclassical approximation* for the system, these supercoherent generalizations provide an *exact*, yet similarly classicized, description. In this way each ICM provides a *supercoherent map* of the Hilbert space $\mathcal{H}$ and the quantum-mechanical Hamiltonian operator H into the target classical phase space Γ_{phys}^H and its associated classical Hamiltonian $\bar{H}$ for a set of multiconfigurational fields $\{x_I, \tilde{x}_I\}$.

The simplest of the IC parametrizations, namely the CIM, provides a classical mapped Hamiltonian $\bar{H}[x_I, \tilde{x}_I]$ which is essentially linear in both sets of coordinates $\{x_I\}$ and $\{\tilde{x}_I\}$. Conversely, the NCCM is linear in the coordinates $\{\tilde{x}_I\}$ but nonlinear in the set $\{x_I\}$. Only the ECCM is intrinsically fully nonlinear in all coordinates. These nonlinear CC parametrizations lead to supercoherent mappings from $\mathcal{H}$ to Γ_{phys}^H which are usually one-to-many rather than one-to-one. Although the resulting non-uniqueness of the CC coordinates is shown to have no effect on physical observables (e.g., expectation values), the resulting topology of the mapped CC phase spaces Γ_{phys}^H has the potential to be rather complicated. Indeed, in geometrical terms, underlying nonlinear equations generally introduce a nontrivial structure to the space of the associated dynamical variables [22].

In the light of the above discussion we now wish to study carefully the classical Hamiltonian $\bar{H}[x_I, \tilde{x}_I]$ and the structure of the associated phase space Γ_{phys}^H induced by each of the three IC parametrizations. Special attention is focused in the present paper on the local algebraic structure of these classical mappings, while a subsequent paper (hereafter referred to as III) addresses their global structure, which is more appropriately addressed in terms of the geometrical properties of the IC phase spaces.

As in I, the Bargmann or holomorphic representation continues to provide a key mathematical tool in our algebraization process. It enables, for example, a bosonic quantum field theory defined in a Hilbert space $\mathcal{H}$ to be mapped into a classical field theory of complex functions in a particular normed space, namely the Bargmann Hilbert space [23–26]. The basic formalism is briefly reviewed in Section II in the context of applications to the single-mode bosonic field theories (e.g., anharmonic oscillators of even order $2K$) studied here via their IC parametrizations. In Section III we then undertake a thorough study of the analytic

and asymptotic properties of all functions needed in the holomorphic representation of the CC parametrizations.

In Section IV we introduce the generating functional from which one may derive expectation values of arbitrary operators within $\mathcal{H}$. The results are illustrated via a thorough discussion of the quartic anharmonic oscillator.

In Section V we also introduce a method by which expectation values of products of individual operators can be computed in the mapped classical phase space Γ^H in terms of the observables (i.e., the expectation values of the individual operators) themselves. Thus, while the classical map of a quantum theory induced by each ICM does indeed provide an equivalent classical mechanics based on the traditional concepts of phase space, Hamiltonian, and flow, the mechanics is not entirely conventional. In particular, for the usual “classical mechanics of pure states” we would have $\overline{BA} = \overline{AB} = \overline{A}\overline{B}$, where the overbar simply represents the observable value. Clearly, in our IC classical maps, an observable value $\overline{A}$ now represents the expectation value of the quantum-mechanical operator A . The formal device which enables us to incorporate the quantal origins of the classical map is the so-called *ICM star product*, whereby the classical IC phase spaces are endowed with a new algebraic structure, by means of which we can write $\overline{AB} = \overline{A} * \overline{B}$. It has the specific property that $\overline{A} * \overline{B} - \overline{B} * \overline{A}$ is a (generalized) Poisson bracket. Commutators of operators in $\mathcal{H}$ are thus mapped into Poisson brackets in Γ^H , thereby endowing the latter with a symplectic structure.

In Section V we also briefly review other theories which introduce the concept of a “star product.” The most important example is the Moyal star product introduced a long time ago. Its generalization is the *deformation theory* which is considered to provide an autonomous road to quantization, i.e., the star product quantization. It is closely related to such topical subjects as the theory of quantum groups. We compare deformation theory with the ICM star product and emphasize their conceptual differences.

In Section VI we proceed to an algebraic analysis of the diagrammatic content of each ICM in terms of the associated emergent tree diagram structures discussed previously [14, 20, 21]. In particular, the special linking and double-linking requirements which are the hallmarks of the NCCM and ECCM, respectively, are given a wholly algebraic interpretation. Finally, our results are summarized and discussed in Section VII.

II. PRELIMINARIES: THE ICM PARAMETRIZATIONS AND THEIR BARGMANN REPRESENTATIONS FOR SINGLE-MODE BOSONIC FIELD THEORIES

The notation of this paper differs slightly from our earlier conventions in I. We believe that the present choices are both more intelligible and logical. Nevertheless, we apologize to the reader for any inconvenience.

We have described in detail in I how the three so-called independent-cluster (IC) methods provide a rather natural hierarchy of parametrizations for arbitrary

quantum-mechanical many-body states $|\Psi\rangle = |\Psi(t)\rangle$ and $\langle\tilde{\Psi}| = \langle\tilde{\Psi}(t)|$ within some appropriate many-body Hilbert space $\mathcal{H}$. They satisfy the Schrödinger equations

$$H|\Psi\rangle = i\frac{\partial}{\partial t}|\Psi\rangle, \quad \langle\tilde{\Psi}|H = -i\frac{\partial}{\partial t}\langle\tilde{\Psi}|. \quad (2.1)$$

As discussed in I (and see also Ref. [14]), the Schrödinger dynamics is reproduced by requiring in *any complete* parametrization of the bra and ket states, that the full action functional,

$$\begin{aligned} \mathcal{A} &\equiv \int_{t_1}^{t_2} dt \langle\tilde{\Psi}(t)| \left(i\frac{\partial}{\partial t} - H \right) |\Psi(t)\rangle \\ &= \mathcal{A}_0 - \int_{t_1}^{t_2} dt \bar{H}, \end{aligned} \quad (2.2)$$

be stationary with respect to all free independent (variational) parameters that fully characterize the states, such that the variations are zero at the two times t_1 and t_2 (usually chosen to be $\pm\infty$). Above, we have introduced the temporal action functional

$$\mathcal{A}_0 \equiv \int_{t_1}^{t_2} dt \langle\tilde{\Psi}(t)| i\frac{\partial}{\partial t} |\Psi(t)\rangle. \quad (2.3)$$

For many purposes it is convenient to choose the normalization such that $\langle\tilde{\Psi}|\Psi\rangle = 1$ for all times t , so that in the usual case where the Hamiltonian is Hermitian, $H = H^\dagger$, we have $\langle\tilde{\Psi}| = \langle\Psi|\Psi\rangle^{-1}\langle\Psi|$, where $\langle\Psi| = (|\Psi\rangle)^\dagger$. Each of the three ICM parametrizations is specified in general with respect to some suitable model state $|0\rangle$, whose key role is that of a *cyclic vector* which separates the algebra of all possible operators in $\mathcal{H}$ into two Abelian subalgebras of multi-configurational creation and destruction operators, $\mathcal{C}$ and $\bar{\mathcal{C}}$, respectively, defined with respect to it. For the purposes of this paper, wherein we consider only single-mode bosonic field theories in which the single-boson creation and destruction operators, $a^\dagger$ and a , respectively, satisfy the usual canonical commutation relations (CCR),

$$[a, a] = [a^\dagger, a^\dagger] = 0, \quad [a, a^\dagger] = I, \quad (2.4)$$

where I is the unit operator, an obvious choice for $|0\rangle$ is the (normalized) “bare vacuum” defined by

$$a|0\rangle = 0, \quad \langle 0|0\rangle = 1. \quad (2.5)$$

Although this is not the only possible choice, it was the choice made in I and we do not consider alternatives to it here.

Each of the three ICM representations now introduces a distinct pair of operators $\{X, \tilde{X}\} \equiv \{X(t), \tilde{X}(t)\}$ which fully parametrize the states $\{|\Psi(t)\rangle, \langle\tilde{\Psi}(t)|\}$, and such that $X \in \mathcal{C}$, $\tilde{X} \in \tilde{\mathcal{C}}$. Thus, in the present case of single-mode bosonic field theory, with $|0\rangle$ as the cyclic vector, we have the general representations,

$$X \equiv \sum_{n=0}^{\infty} \frac{X_n}{\sqrt{n!}} (a^\dagger)^n; \quad \tilde{X} \equiv \sum_{n=0}^{\infty} \frac{\tilde{X}_n}{\sqrt{n!}} a^n. \quad (2.6)$$

A distinctive common feature of all three ICM representations, as shown in I, is that the c -number coefficients $\{X_n(t), \tilde{X}_n(t)\}$ obey the generic *canonical equations of motion*,

$$i \frac{dX_n}{dt} = \frac{\partial \bar{H}}{\partial \tilde{X}_n}; \quad -i \frac{d\tilde{X}_n}{dt} = \frac{\partial \bar{H}}{\partial X_n}, \quad (2.7)$$

where $\bar{H} \equiv \langle\tilde{\Psi}(t)| H |\Psi(t)\rangle \equiv \bar{H}[X_n, \tilde{X}_n]$ is the c -number energy expectation value.

In the CIM the representations are $\{X, \tilde{X}\} \rightarrow \{F, \tilde{F}\}$, where we choose to define

$$\begin{aligned} |\Psi\rangle &= F|0\rangle, & \langle\tilde{\Psi}| &= \langle 0| \tilde{F}; \\ F &\equiv f(a^\dagger) = \sum_{n=0}^{\infty} f_n (a^\dagger)^n, & \tilde{F} &\equiv \tilde{f}(a) = \sum_{n=0}^{\infty} \tilde{f}_n a^n. \end{aligned} \quad (2.8)$$

For practical reasons, in both this and the subsequent coupled cluster (CC) cases the amplitudes are actually normalized differently from the convention of Eq. (2.6), so that, in general, we write $X_n = \sqrt{n!} x_n$, $\tilde{X}_n = \sqrt{n!} \tilde{x}_n$. Thus, we do not need always to carry along the square roots of factorials in the algebraic expressions. The difference in normalization shows up in the canonical equations of motion, which have an extra factor of $(n!)^{-1}$ in the right-hand sides when written in terms of the amplitudes $\{x_n, \tilde{x}_n\}$, in comparison with Eqs. (2.7).

We shall adopt the convention, as exemplified by Eq. (2.8), that while the operators are usually denoted by capital letters, their Bargmann representations as functions of the complex variable are written in lower case.

For the NCCM the comparable choice is $\{X, \tilde{X}\} \rightarrow \{S, \tilde{S}\}$, where

$$\begin{aligned} |\Psi\rangle &= \kappa e^S |0\rangle, & \langle\tilde{\Psi}| &= \frac{1}{\kappa} \langle 0| \tilde{S} e^{-\tilde{S}}, \\ S &\equiv s(a^\dagger) = \sum_{n=1}^{\infty} s_n (a^\dagger)^n, & \tilde{S} &\equiv \tilde{s}(a) = 1 + \sum_{n=1}^{\infty} \tilde{s}_n a^n. \end{aligned} \quad (2.9)$$

We note in particular the choices $s_0 = 0$ and $\tilde{s}_0 = 1$. Finally, in the ECCM we have $\{X, \tilde{X}\} \rightarrow \{\Sigma, \tilde{\Sigma}\}$, where

$$\begin{aligned}
 |\Psi\rangle &= \kappa e^S |0\rangle, & \langle\tilde{\Psi}| &= \frac{1}{\kappa} \langle 0| e^{\tilde{S}} e^{-S}, & \tilde{S} &\equiv e^{\tilde{S}}, \\
 \Sigma |0\rangle &\equiv Q e^{\tilde{S}} S |0\rangle, & Q &\equiv I - |0\rangle\langle 0|, \\
 \Sigma &\equiv \sigma(a^\dagger) = \sum_{n=1}^{\infty} \sigma_n (a^\dagger)^n, & \tilde{\Sigma} &\equiv \tilde{\sigma}(a) = \sum_{n=1}^{\infty} \tilde{\sigma}_n a^n.
 \end{aligned} \tag{2.10}$$

We note again the particular choices $\sigma_0 = \tilde{\sigma}_0 = 0$. Equations (2.9) and (2.10) readily yield the inverse relationships between the ECCM coefficients $\{\sigma_n\}$ and the NCCM coefficients $\{\tilde{\sigma}_n\}$,

$$\sigma_n = \frac{1}{n!} \langle 0| a^n \tilde{S} S |0\rangle, \quad s_n = \frac{1}{n!} \langle 0| a^n e^{-\tilde{S}} \Sigma |0\rangle, \quad n \geq 1. \tag{2.11}$$

In both the NCCM and the ECCM the normalization condition $\langle\tilde{\Psi}|\Psi\rangle = 1$ is explicit.

The c -number scale factor $\kappa = \kappa(t)$ is necessary only for time-dependent states. However, it has no effect on the equations of motion of the CCM amplitudes, because it can be gauged away by the temporal transformation

$$H \rightarrow H - i \frac{d}{dt} \ln \kappa, \tag{2.12}$$

with the constraint $i(d/dt) \ln \kappa = \langle 0| H e^S |0\rangle$. Thus we may simply adopt the convention $\kappa = 1$, so that the CCM states also satisfy the intermediate normalization condition, $\langle 0|\Psi\rangle = 1 = \langle\tilde{\Psi}|\Psi\rangle$. However, it is evident that the stationary value of the action functional to be discussed in a subsequent paper (and see also I) does depend on the convention. In particular, in both the CCM cases (NCCM and ECCM) the temporal part is the phase

$$\varphi_B \equiv \mathcal{A}_0^{CCM} = \mathcal{A}_0 - i \ln \kappa(t) \Big|_{t_1}^{t_2}. \tag{2.13}$$

This is a phase variable whose real part in an adiabatic change of an eigenstate of the Hamiltonian turns out to be precisely the geometric Berry's phase (see, e.g., Ref. [27]). In our case φ_B can have an imaginary part due to the special CCM normalization conventions, but for closed loops in the parameter space the imaginary part vanishes.

The CCR of Eq. (2.4) may be specifically realized in the so-called Bargmann Hilbert space, characterized by the algebra

$$a^\dagger \rightarrow z; \quad a \rightarrow d/dz, \tag{2.14}$$

of the complex variable z and its derivative. Arbitrary states in the Fock space now

have the equivalent Bargmann (or holomorphic) representations, which satisfy such typical relations as

$$\begin{aligned} f(a) g(a^\dagger) |0\rangle &\equiv h(a^\dagger) |0\rangle \Leftrightarrow f\left(\frac{d}{dz}\right) g(z) = h(z), \\ \langle 0| f(a) g(a^\dagger) &\equiv \langle 0| \tilde{h}(a) \Leftrightarrow g\left(\frac{d}{dz}\right) f(z) = \tilde{h}(z). \end{aligned} \quad (2.15)$$

The original single-mode bosonic field theory is thereby mapped into the corresponding (classical) field theory of a complex function in a certain normed space, namely the Bargmann Hilbert space [23–26]. As has been described in more detail in I, we may now construct various specific forms for the inner product between two arbitrary states,

$$\begin{aligned} |g\rangle &\equiv g(a^\dagger) |0\rangle, \quad \langle f^*| \equiv \langle 0| f(a) = [\langle f^*(a^\dagger) |0\rangle]^\dagger = (|f^*\rangle)^\dagger; \\ g(z) &= \sum_{n=0}^{\infty} g_n z^n, \quad f(z) = \sum_{n=0}^{\infty} f_n z^n. \end{aligned} \quad (2.16)$$

These include the forms,

$$\langle f^* | g \rangle = f\left(\frac{d}{dz}\right) g(z) \Big|_{z=0} = g\left(\frac{d}{dz}\right) f(z) \Big|_{z=0} \quad (2.17a)$$

$$= \sum_{n=0}^{\infty} n! f_n g_n \quad (2.17b)$$

$$= \frac{1}{\pi} \int d^2z e^{-|z|^2} f(z) g(z^*) = \frac{1}{\pi} \int d^2z e^{-|z|^2} f(z^*) g(z), \quad (2.17c)$$

where the integrations in Eq. (2.17c) extend over the entire complex z -plane. Another form that turns out to be very useful is based on the Fourier representation, if it exists, of one of the functions, say $f(z)$,

$$f(z) = \int_P \frac{d\zeta}{2\pi} e^{i\zeta z} f_F(\zeta), \quad (2.18)$$

where P is a suitable path in the complex plane and is given by

$$\langle f^* | g \rangle = \int_P \frac{d\zeta}{2\pi} f_F(\zeta) g(i\zeta). \quad (2.17d)$$

It is important to recall that if the two states $\langle f^*|$ and $|g\rangle$ are normalizable then Eq. (2.17c) implies that both $f(z)$ and $g(z)$ must be *holomorphic* or *entire* functions of order $\rho \leq 2$ (and of type $\tau \leq \frac{1}{2}$ in the limiting case $\rho = 2$). It is for precisely this reason that the Bargmann representation is known equivalently as the holomorphic

representation. For such functions it is also relatively straightforward to prove that each of the alternative versions (2.17a)–(2.17d) for the norm $\langle f^* | g \rangle$ yields the same *convergent* result. On the other hand, when the Hilbert space $\mathcal{H}$ of normalizable wave functions is enlarged to a more general linear vector space which includes states of infinite norm (in the conventional metrics), differences between the four forms of Eqs. (2.17a)–(2.17d) arise. In particular, meaning needs to be attached to the otherwise divergent expressions which automatically arise as a consequence. We saw in I that just such an extension of $\mathcal{H}$ is necessitated by the two CCM parametrizations of the state vectors. In this context the Bargmann-space representation techniques were shown in I to provide a definite regularization procedure for handling such divergent expressions, each of which typically arises from a formal expansion of certain otherwise exact (and convergent) integrals.

If we define the average value of an arbitrary operator $O = O(a^\dagger, a)$ as

$$\langle O \rangle \equiv \bar{O} \equiv \langle \tilde{\Psi} | O | \Psi \rangle, \quad (2.19)$$

we may now consider the Bargmann-space representation of $\bar{O}$ for each of the three ICM parametrizations. Thus, first, for the case of the CIM parametrization we clearly have

$$\begin{aligned} \bar{O} &= \langle 0 | f^*(a) O(a^\dagger, a) f(a^\dagger) | 0 \rangle / \langle 0 | f^*(a) f(a^\dagger) | 0 \rangle \\ &= \left[f^* \left(\frac{d}{dz} \right) O \left(z, \frac{d}{dz} \right) f(z) \right]_{z=0} / \left[f^* \left(\frac{d}{dz} \right) f(z) \right]_{z=0} \\ &= \tilde{f} \left(\frac{d}{dz} \right) O \left(z, \frac{d}{dz} \right) f(z) \Big|_{z=0}. \end{aligned} \quad (2.20)$$

Second, the counterpart to Eq. (2.20) for the NCCM parametrization is

$$\begin{aligned} \bar{O} &= \langle 0 | \tilde{s}(a) e^{-s(a^\dagger)} O(a^\dagger, a) e^{s(a^\dagger)} | 0 \rangle \\ &= \tilde{s} \left(\frac{d}{dz} \right) e^{-s(z)} O \left(z, \frac{d}{dz} \right) e^{s(z)} \Big|_{z=0}. \end{aligned} \quad (2.21)$$

If we now formally expand $O(z, d/dz)$ as an ordered multinomial in z and d/dz , we may insert a unit operator of the form $I = e^{s(z)} e^{-s(z)}$ between every pair of adjacent operators in the ensuing expansion. We may then use the trivial relation

$$e^{-s(z)} \frac{d}{dz} e^{s(z)} = \frac{d}{dz} + s'(z) \quad (2.22)$$

to rewrite Eq. (2.21) in the equivalent NCCM form,

$$\bar{O} = \tilde{s} \left(\frac{d}{dz} \right) O \left(z, \frac{d}{dz} + s'(z) \right) \Big|_{z=0}. \quad (2.23)$$

Finally, the ECCM parametrization yields the average value,

$$\begin{aligned}\bar{O} &= \langle 0 | e^{\tilde{\sigma}(a)} e^{-s(a^\dagger)} O(a^\dagger, a) e^{s(a^\dagger)} | 0 \rangle \\ &= e^{\tilde{\sigma}(d/dz)} e^{-s(z)} O\left(z, \frac{d}{dz}\right) e^{s(z)} \Big|_{z=0}.\end{aligned}\quad (2.24)$$

As in the previous NCCM case, this may be rewritten as

$$\bar{O} = e^{\tilde{\sigma}(d/dz)} O\left(z, \frac{d}{dz} + s'(z)\right) e^{-\tilde{\sigma}(d/dz)} 1 \Big|_{z=0}, \quad (2.25)$$

where in inserting the last factor we use that $\tilde{\sigma}(0) = \tilde{\sigma}_0 = 0$. The operator $O[z, d/dz + s'(z)]$ may once again be formally expanded as an ordered multinomial in z and $[d/dz + s'(z)]$, and a unit operator of the form $I = e^{-\tilde{\sigma}(d/dz)} e^{\tilde{\sigma}(d/dz)}$ may be inserted between every pair of adjacent operators in the resulting expansion. Use of the simple relation,

$$e^{\tilde{\sigma}(d/dz)} z e^{-\tilde{\sigma}(d/dz)} = z + \tilde{\sigma}'\left(\frac{d}{dz}\right), \quad (2.26)$$

then readily yields the expression

$$\bar{O} = O\left[z + \tilde{\sigma}'\left(\frac{d}{dz}\right), \frac{d}{dz} + e^{\tilde{\sigma}(d/dz)} s'(z) e^{-\tilde{\sigma}(d/dz)}\right] \Big|_{z=0}. \quad (2.27)$$

The definition in Eq. (2.10) yields the equivalent Bargmann-space relation,

$$\sigma(z) = e^{\tilde{\sigma}(d/dz)} s(z) - e^{\tilde{\sigma}(d/dz)} s(z) \Big|_{z=0}, \quad (2.28)$$

by making use of Eq. (2.15). Thus we have the relation

$$\sigma'(z) = e^{\tilde{\sigma}(d/dz)} s'(z), \quad (2.29)$$

and at first sight it is tempting to substitute this relation directly into Eq. (2.27). However, this is clearly incorrect since in Eq. (2.29) the derivatives in the exponent are not supposed to act beyond the factor $s'(z)$, as they are in Eq. (2.27). Thus, despite Eq. (2.29),

$$\sigma'(z) f(z) \neq e^{\tilde{\sigma}(d/dz)} s'(z) f(z), \quad (2.30)$$

for general functions of $f(z)$ other than constants. Nevertheless, by inverting Eq. (2.29), we may write, denoting for convenience $z \rightarrow iz$,

$$\begin{aligned}
 s'(iz) &= e^{-\partial(-id/dz)} \sigma'(iz) \\
 &= e^{-\partial(-id/dz)} \int_{-\infty}^{\infty} \frac{dx}{2\pi} \int_{-\infty}^{\infty} dy e^{-ix(y-z)} \sigma'(iy) \\
 &= \int_{-\infty}^{\infty} \frac{dx}{2\pi} \int_{-\infty}^{\infty} dy e^{-ix(y-z)} e^{-\partial(x)} \sigma'(iy). \tag{2.31}
 \end{aligned}$$

Last, we may rewrite Eq. (2.31) as

$$e^{\partial(d/dz)} s'(z) e^{-\partial(d/dz)} = \int_{-\infty}^{\infty} \frac{dx}{2\pi} \int_{-\infty}^{\infty} dy e^{-ix(y+iz)} \sigma'(iy) e^{\partial(x+d/dz) \cdots \partial(x) - \partial(d/dz)}, \tag{2.32}$$

in which form it may be substituted directly into Eq. (2.27). We observe that the ECCM expression for $\bar{O}$ cannot be given in an equally straightforward manner in terms of its natural variables as in the NCCM case. These last expressions are clearly formal until the convergence of the integrations is confirmed.

Although the NCCM and ECCM average-value expressions of Eq. (2.23) and Eqs. (2.27) and (2.32), respectively, are formally exact, they are cumbersome to use in practice for anything other than the evaluation of relatively low-order terms. Nevertheless, for present purposes we are more concerned with the exact qualitative properties of the various IC parametrizations. We are therefore more interested in the analytic properties of the particular Bargmann amplitudes which characterize each parametrization, and to this end we will need to focus special attention on their asymptotic properties. In order to be as specific as possible we shall actually specialize the remaining discussion to anharmonic oscillators of order $2K$, where $K=2, 3, \dots$, in one space dimension $x \in (-\infty, \infty) \equiv \mathbf{R}$.

III. ASYMPTOTICS OF THE ICM BARGMANN AMPLITUDES FOR ANHARMONIC OSCILLATOR SYSTEMS

The general Hamiltonian is specified in terms of the coordinate operator $\hat{x}$ and its canonically conjugate momentum operator $\hat{p}$ as

$$H = \frac{1}{2} \hat{p}^2 + \frac{1}{2} \hat{x}^2 + U(\sqrt{2} \hat{x}). \tag{3.1}$$

Its energy eigenstates $|\Psi_n\rangle$ and eigenvalues E_n satisfy the Schrödinger equation,

$$H |\Psi_n\rangle = E_n |\Psi_n\rangle. \tag{3.2}$$

In the usual coordinate-space representation, $\langle x | \Psi_n \rangle \equiv \psi_n(x)$, where $\hat{x} \rightarrow x$, $\hat{p} \rightarrow -id/dx$, we require that $\psi(x) \in L^2([-\infty, \infty], \mathbf{C})$. We assume the states $|\Psi_n\rangle$ and wave functions $\psi_n(x)$ to be orthonormalized in the usual way. The one-body

Schrödinger Hamiltonian of Eq. (3.1) may be equivalently specified as the single-mode bosonic field theory with Hamiltonian,

$$H(a^\dagger, a) = H = \frac{1}{2} + a^\dagger a + U(a^\dagger + a), \quad (3.3)$$

in terms of the operators a and $a^\dagger$ defined as

$$a \equiv 2^{-1/2}(\hat{x} + i\hat{p}), \quad a^\dagger \equiv 2^{-1/2}(\hat{x} - i\hat{p}), \quad (3.4)$$

which satisfy the bosonic CCR of Eq. (2.4).

In the Bargmann representation of Eq. (2.14), the eigenstates $|\Psi_n\rangle$ have the CIM Fock-space parametrization,

$$|\Psi_n\rangle = f^n(a^\dagger) |0\rangle, \quad (3.5)$$

and the Bargmann eigenstates $f^n(z)$ corresponding to the Schrödinger eigenstates $\psi_n(x)$ then obey the ordinary differential equation in the complex z -plane,

$$\left[\frac{1}{2} + z \frac{d}{dz} + U\left(z + \frac{d}{dz}\right) \right] f^n(z) = E_n f^n(z). \quad (3.6)$$

If $f^n(z)$ is written in the form

$$f^n(z) \equiv \exp\left(-\frac{1}{2}z^2\right) \phi^n(z), \quad (3.7)$$

Eq. (3.6) can be rewritten in the equivalent form,

$$\left[\frac{1}{2} - z^2 + z \frac{d}{dz} + U\left(\frac{d}{dz}\right) \right] \phi^n(z) = E_n \phi^n(z). \quad (3.8)$$

For the specific case of the anharmonic oscillator potential,

$$U(\sqrt{2}x) = kx^{2K}; \quad k > 0, \quad K = 2, 3, \dots, \quad (3.9)$$

to which we henceforth restrict ourselves, Eq. (3.8) takes the form

$$\left(\frac{d}{dz}\right)^{2K} \phi^n(z) = \frac{2^K}{k} \left(-z \frac{d}{dz} + z^2 + E_n - \frac{1}{2}\right) \phi^n(z). \quad (3.10)$$

The corresponding Schrödinger equation for $\psi_n(x)$ is

$$\left(-\frac{1}{2} \frac{d^2}{dx^2} + \frac{1}{2} x^2 + kx^{2K}\right) \psi_n(x) = E_n \psi_n(x). \quad (3.11)$$

It is trivial to show in the usual WKB fashion from Eq. (3.11) that the leading asymptotic behaviour of $\psi_n(x)$ is

$$\psi_n(x) \propto \exp\left(-\frac{\sqrt{2k}}{(K+1)} |x|^{K+1}\right), \quad x \rightarrow \pm\infty. \quad (3.12)$$

A similar WKB analysis of the asymptotic behaviour of $\phi^n(z)$ as $|z| \rightarrow \infty$ can also be performed on Eq. (3.10). The interested reader is referred to Appendix B of I for further details. Alternatively, we also showed in I that there exists a Fourier-like relationship between $\phi^n(z)$ and $\psi_n(x)$,

$$\phi^n(z) = \pi^{-1/4} \int_{-\infty}^{\infty} dx \exp(\sqrt{2}zx - \frac{1}{2}x^2) \psi_n(x), \quad (3.13)$$

from which it is clear that $\phi^n(z)$ is an entire function of z . Use of Eq. (3.12) and the saddle-point method in Eq. (3.13) easily shows that along the real axis the functions $\phi^n(z)$ behave asymptotically as

$$\phi^n(x) \propto \exp(b|x|^v), \quad x \rightarrow \pm \infty, \quad (3.14)$$

where

$$v \equiv \frac{(K+1)}{K}, \quad b \equiv \frac{\sqrt{2}}{v} \left(\frac{1}{k} \right)^{1/(2K)}. \quad (3.15)$$

Thus, the functions $\phi^n(z)$ are entire functions of fractional order v , where $1 < v < 2$. Furthermore, along the imaginary axis the functions $\phi^n(z)$ oscillate and have an infinite sequence of zeros, with an amplitude function which approaches zero with leading asymptotic behaviour,

$$\phi^n(iy) \propto \exp(-\alpha|y|^v), \quad y \rightarrow \pm \infty, \quad (3.16)$$

where

$$\alpha \equiv b \sin\left(\frac{\pi}{2K}\right) > 0. \quad (3.17)$$

Thus, the functions $\phi^n(iy) \in L^2([-\infty, \infty], \mathbb{C})$. The zeros z_m of $\phi^n(z)$, and hence also of $f^n(z)$, asymptotically approach the imaginary axis, $z_m \rightarrow \pm iy_m$, with a distribution

$$y_m \xrightarrow{m \rightarrow \infty} \left[\frac{\pi}{b} \sec\left(\frac{\pi}{2K}\right) \right]^{1/v} m^{1/v}. \quad (3.18)$$

It is also convenient for later purposes to introduce a Fourier transform $f_{\mathbb{F}}^n$ of f^n along the real axis, defined as

$$f_{\mathbb{F}}^n(z) \equiv \int_{-\infty}^{\infty} dx e^{-izx} f^n(x). \quad (3.19)$$

Just as $f^n(z)$ is an entire function of z of order 2 and type $\frac{1}{2}$, it turns out that so

is $f_F^n(z)$. Furthermore, along the real axis it decreases asymptotically to zero with leading behaviour,

$$f_F^n(x) \propto e^{-x^2/2}, \quad x \rightarrow \pm \infty. \quad (3.20)$$

The inverse of Eq. (3.19) may thus be written for arbitrary z as

$$f^n(z) = \int_{-\infty}^{\infty} \frac{dx}{2\pi} e^{izx} f_F^n(x). \quad (3.21)$$

If $f_F^n(z)$ is further written as the product,

$$f_F^n(z) \equiv e^{-z^2/2} \chi^n(z), \quad (3.22)$$

then the definitions (3.7) and (3.19) immediately yield the relation

$$\chi^n(z) = \int_{-\infty}^{\infty} dx e^{-x^2/2} \phi^n(x - iz). \quad (3.23)$$

By either writing $\phi^n(x - iz)$ in terms of its Fourier transform, or by making a Taylor expansion of it about the point $-iz$, it is straightforward to show that Eq. (3.23) can be written in the equivalent form,

$$\chi^n(z) = \sqrt{2\pi} \exp\left(-\frac{1}{2} \frac{d^2}{dz^2}\right) \phi^n(-iz). \quad (3.24)$$

Furthermore, by using Eq. (3.13), we may also rewrite Eq. (3.23) so as to express $\chi^n(z)$ in terms of $\psi_n(x)$ as

$$\chi^n(z) = 2^{1/2} \pi^{1/4} \int_{-\infty}^{\infty} dx \exp(-i\sqrt{2}zx + \frac{1}{2}x^2) \psi_n(x), \quad (3.25)$$

which may be compared with Eq. (3.13). Finally, by making use of the Schrödinger equation (3.11), it is easy to show from Eq. (3.25) that the function $\chi^n(iz)$ satisfies the differential equation

$$\left(\frac{d}{dz}\right)^{2K} \chi^n(iz) = \frac{2K}{k} \left(z \frac{d}{dz} + z^2 + E_n + \frac{1}{2}\right) \chi^n(iz), \quad (3.26)$$

which may be compared with Eq. (3.10).

We may again use the saddle-point method in Eq. (3.25), together with Eq. (3.12), to show that along the imaginary axis the functions $\chi^n(z)$ behave asymptotically as

$$\chi^n(iy) \propto \exp(b|y|^v), \quad y \rightarrow \pm \infty, \quad (3.27)$$

where the constants v and b are as defined previously in Eq. (3.15). We see that just

like the functions $\phi''(z)$, so the functions $\chi''(z)$ are also entire functions of fractional order ν . Since the functions $\chi''(x)$, $x \in \mathbf{R}$, are Fourier transforms of square-integrable functions, they must themselves be square-integrable: $\chi''(x) \in L^2([-\infty, \infty], \mathbf{C})$. This property can be used in a WKB analysis to show that asymptotically along the real axis, the functions $\chi''(z)$ oscillate and again have an infinite sequence of zeros, with an amplitude function which approaches zero with leading asymptotic behaviour,

$$\chi''(x) \propto \exp(-\alpha |x|^\nu), \quad x \rightarrow \pm \infty, \quad (3.28)$$

with $\alpha > 0$ as given in Eq. (3.17).

The bra-state Schrödinger equation for $\tilde{f}^n$ may be written in terms of an arbitrary function $\zeta(z)$ as

$$\langle 0 | \tilde{f}^n(a) H(a^\dagger, a) \zeta(a^\dagger) | 0 \rangle = E_n \langle 0 | \tilde{f}^n(a) \zeta(a^\dagger) | 0 \rangle, \quad (3.29)$$

or, equivalently, from Eq. (2.15) as

$$\tilde{f}^n \left(\frac{d}{dz} \right) H \left(z, \frac{d}{dz} \right) \zeta(z) \Big|_{z=0} = E_n \tilde{f}^n \left(\frac{d}{dz} \right) \zeta(z) \Big|_{z=0}. \quad (3.30)$$

By writing $\tilde{f}^n$ in terms of its Fourier transform $\tilde{f}_F^n$ exactly as in Eq. (3.21), we may rewrite Eq. (3.30) in the form

$$\int_{-\infty}^{\infty} \frac{dx}{2\pi} \tilde{f}_F^n(x) e^{ix(d/dz)} H \left(z, \frac{d}{dz} \right) \zeta(z) \Big|_{z=0} = E_n \int_{-\infty}^{\infty} \frac{dx}{2\pi} \tilde{f}_F^n(x) e^{ix(d/dz)} \zeta(z) \Big|_{z=0}, \quad (3.31)$$

and hence as

$$\int_{-\infty}^{\infty} \frac{dx}{2\pi} \tilde{f}_F^n(x) H \left(z + ix, \frac{d}{dz} \right) \zeta(z + ix) \Big|_{z=0} = E_n \int_{-\infty}^{\infty} \frac{dx}{2\pi} \tilde{f}_F^n(x) \zeta(ix). \quad (3.32)$$

Finally, by using the simple relation $(d/dz) \zeta(z + ix) = -i(d/dx) \zeta(z + ix)$, we have the relation

$$\int_{-\infty}^{\infty} \frac{dx}{2\pi} \tilde{f}_F^n(x) H \left(ix, -i \frac{d}{dz} \right) \zeta(ix) = E_n \int_{-\infty}^{\infty} \frac{dx}{2\pi} \tilde{f}_F^n(x) \zeta(ix). \quad (3.33a)$$

for an arbitrary function $\zeta(z)$, and where, as always, we understand the differential operator d/dx to act to the right. However, we have been cautious enough to allow the derivative operator d/dz in $H(z, d/dz)$ to act also on the z 's within H itself. Thus, we do not require the Hamiltonian to be normal ordered. On the other hand, we may also let the differential operator d/dx act to the left by partial integration.

In this way, since $\zeta(z)$ is arbitrary, we may write the above result in the equivalent form,

$$\tilde{f}_F^n(x) H\left(ix, i \frac{\tilde{d}}{dx}\right) = E_n \tilde{f}_F^n(x), \quad (3.33b)$$

in a self-evident notation where the operator $(\tilde{d}/dx)$ acts on functions of x to the left of itself. This latter equation may be compared with the corresponding Schrödinger equation for the ket-state Bargmann representative $f^n(ix)$,

$$H\left(ix, -i \frac{d}{dx}\right) f^n(ix) = E_n f^n(ix). \quad (3.34)$$

We turn now to the NCCM for which the operators which parametrize the states $|\Psi_n\rangle$ and $\langle\tilde{\Psi}_n|$ are specified as S^n and $\tilde{S}^n$. They are defined as in Eq. (2.9), with the usual choice $\kappa=1$ for the c-number scale factor. By using Eq. (2.15), a comparison of Eqs. (2.8) and (2.9) shows that the Bargmann representation for $\tilde{s}^n(z)$ is

$$\tilde{s}^n(z) = f^n\left(\frac{d}{dz}\right) \tilde{f}^n(z). \quad (3.35)$$

The normalization $\langle\tilde{\Psi}_n|\Psi_n\rangle = 1$ now implies that

$$\tilde{f}^n(z) = f^{n*}(z) / \left[f^n\left(\frac{d}{dz}\right) f^{n*}(z) \right]_{z=0}, \quad (3.36)$$

where the asterisk denotes complex conjugation of the functional form, as usual. This corresponds to the normalization condition

$$\delta_{m,n} = \langle\tilde{\Psi}_m|\Psi_n\rangle = \int_{-\infty}^{\infty} \frac{dx}{2\pi} \tilde{f}_F^m(x) f^n(ix). \quad (3.37)$$

By making use of Eqs. (3.7), (3.13) and the definition (3.21) as applied to $\tilde{f}^n$, we may now readily rewrite Eq. (3.35) in the form

$$\tilde{s}^n(z) = 2^{-1} \pi^{-5/4} \int_{-\infty}^{\infty} dx e^{-x^2/2} \psi_n(x) \int_{-\infty}^{\infty} dy e^{(y^2/2 + \sqrt{2}ixy + izy)} \tilde{f}_F^n(y). \quad (3.38)$$

By making further use of Eqs. (3.22) and (3.25), we may express $\tilde{s}^n(z)$ wholly in terms of $\psi_n(x)$ and $\tilde{\psi}_n(x) \equiv \langle\tilde{\Psi}_n|x\rangle \equiv \psi_n^*(x)/\langle\Psi_n|\Psi_n\rangle$ as

$$\tilde{s}^n(z) = \int_{-\infty}^{\infty} dx \tilde{\psi}_n\left(x + \frac{z}{2\sqrt{2}}\right) \psi_n\left(x - \frac{z}{2\sqrt{2}}\right) e^{xz/\sqrt{2}}. \quad (3.39)$$

For later purposes we shall find it useful to generalize the function $\tilde{s}^n(z)$, which

relates to the NCCM parametrization of a single energy eigenstate, to a function $\tilde{s}^{mn}(z)$ defined by analogy with Eq. (3.39) as

$$\tilde{s}^{mn}(z) \equiv \int_{-\infty}^{\infty} dx \tilde{\psi}_m \left(x + \frac{z}{2\sqrt{2}} \right) \psi_n \left(x - \frac{z}{2\sqrt{2}} \right) e^{xz/\sqrt{2}}, \quad (3.40)$$

in terms of a pair of eigenstates, and such that $\tilde{s}^{nn}(z) = \tilde{s}^n(z)$. The orthonormality condition $\langle \tilde{\Psi}_m | \Psi_n \rangle = \delta_{m,n}$ immediately implies that

$$\tilde{s}^{mn}(0) = \delta_{m,n}. \quad (3.41)$$

We also note that since the ground-state wave function $\psi_0(x)$ has no nodes on the real axis (except at infinity), the function $\tilde{s}^{00}(z)$ has no zeros on the real axis (except at most at infinity). By analogy with Eq. (3.35), the function $\tilde{s}^{mn}(z)$ may also be written in the form

$$\tilde{s}^{mn}(z) = f^n \left(\frac{d}{dz} \right) \tilde{f}^m(z). \quad (3.42)$$

Furthermore, by writing the Fourier transform $\tilde{s}_F^{mn}$ of $\tilde{s}^{mn}$ along the real axis as

$$\tilde{s}_F^{mn}(z) \equiv \int_{-\infty}^{\infty} dx e^{-izx} \tilde{s}^{mn}(x), \quad (3.43)$$

and by writing $\tilde{f}^m(z)$ in Eq. (3.42) in terms of its own Fourier transform $\tilde{f}_F^m$, defined in exact analogy with Eq. (3.21), we have immediately that

$$\tilde{s}_F^{mn}(z) = \tilde{f}_F^m(z) f^n(iz) = \tilde{\chi}^m(z) \phi^n(iz), \quad (3.44)$$

where in the latter equality we have made use of Eq. (3.7) and the analogue of Eq. (3.22) for $\tilde{f}_F^m$ in terms of $\tilde{\chi}_m$. We thus have that the functions $\tilde{s}_F^{mn}(z)$ are entire functions of z of fractional order ν . Equations (3.16) and (3.28) show that along the real axis they decrease to zero with leading asymptotic behaviour,

$$\tilde{s}_F^{mn}(x) \propto \exp(-2\alpha |x|^\nu), \quad x \rightarrow \pm \infty. \quad (3.45)$$

The inverse of Eq. (3.43), defined along the real axis,

$$\tilde{s}^{mn}(z) = \int_{-\infty}^{\infty} \frac{dx}{2\pi} e^{izx} \tilde{s}_F^{mn}(x), \quad (3.46)$$

therefore exists for all values of z as an entire function.

A simple saddle-point analysis of Eq. (3.46) readily shows that along the imaginary axis the leading asymptotic behaviour is

$$\tilde{s}^{mn}(iy) \propto \exp(c |y|^{K+1}), \quad y \rightarrow \pm \infty, \quad (3.47)$$

where

$$c \equiv \frac{\sqrt{k}}{(K+1)} 2^{-3K/2} \left[\operatorname{cosec} \left(\frac{\pi}{2K} \right) \right]^K. \quad (3.48)$$

Thus, $\tilde{s}^{mn}(z)$ is an entire function of integral order $(K+1)$, as are also the Schrödinger wave functions $\psi_n(z)$. Finally, we can also show (and see Appendix C of I) that along the real axis the functions $\tilde{s}^{mn}(x)$ approach zero asymptotically with leading behaviour given by

$$\tilde{s}^{mn}(x) \propto \exp \left(-\frac{\sqrt{k}}{(K+1)} 2^{-3K/2} |x|^{K+1} \right), \quad x \rightarrow \pm \infty. \quad (3.49)$$

By means of Eq. (3.37) it is also readily verified that the sets of functions $\{\phi^n(ix)\}$ and $\{\tilde{\chi}^n(x)\}$ for $x \in \mathbf{R}$ are *biorthonormal*, i.e.,

$$\int_{-\infty}^{\infty} dx \tilde{\chi}^m(x) \phi^n(ix) = \delta_{m,n}. \quad (3.50)$$

For later purposes we shall also need the analytic and asymptotic properties of the two ratio functions,

$$r_n(z) \equiv f^n(z)/f^0(z) \quad (3.51)$$

and

$$\tilde{r}_{mn}(z) \equiv \tilde{s}^{mn}(z)/\tilde{s}^{00}(z). \quad (3.52)$$

These clearly hinge upon the dependence of $f^n(z)$ and $\tilde{s}^{mn}(z)$ on the energy eigenvalues of the wave functions involved in their definitions. It is not difficult to show that the specific incorporation of the dependence on the energy eigenvalues does not change the leading asymptotic behaviour of the functions $f^n(z)$ and $\tilde{s}^{mn}(z)$. Thus, in the limit $|z| \rightarrow \infty$ the above functions $r_n(z)$ and $\tilde{r}_{mn}(z)$ approach constant values, which result is important for the existence of their generalized Fourier transforms. We relegate the details of the investigation to Appendix A.

After considering the amplitude $\tilde{s}(z)$, we turn next to the remaining amplitude which characterizes the NCCM parametrization, namely $s(z)$. We have already indicated above (and see I for further details) that the Bargmann amplitudes $f^n(z)$ which characterize the stationary energy eigenstates have an infinite number of zeros for the anharmonic oscillator potentials under consideration, and that the zeros have accumulation points on the imaginary axis at $\pm i\infty$. Hence, since $s(z) \equiv \ln f(z)$, the function $s(z)$ generally has an infinite number of logarithmic branch point singularities. Thus, the function $s(z)$ is not an entire function, and whenever $s(z)$ is considered for values of z on the imaginary axis, for example, we must understand that at least an infinitesimal shift or rotation away from the imaginary axis is implied. Following the discussion in I, we may, for example,

assume that the function $s(z)$ is parametrized through its values on a straight line L passing through the origin and inclined in the direction $\eta = \exp(i\phi)$ such that L does not overlap any of the branch points. For the ground state of the anharmonic oscillator of order $2K$ the angle ϕ must lie in the range $0 < |\phi - \pi/2| < \pi/2(K+1)$. The whole of the function $s(z)$ can then in principle be constructed by analytic continuation away from the line L .

It will become obvious in the next section that the line L on which $s(z)$ is parametrized does not even have to pass through the origin. In addition to the constraint on the slope, it is only required that it does not go through any of the zeros of $f(z)$. Because of the facts that the distant zeros must lie asymptotically on the imaginary axis and that the density of zeros of an entire function of fractional order ν is restricted by the relation $N(R) \lesssim \text{const} \times R^\nu$, where $N(R)$ is the number of zeros in a circle of radius R [28], there always exist such possible routes for the line L . In fact almost all routes are allowed; the forbidden ones have measure zero. The different lines L away from which the function $s(z)$ is analytically continued correspond to different charts describing the coupled-cluster manifold around a given point (and see the discussion in the subsequent paper III). It may also be possible to generalize the parametrization to curved non-self-intersecting contours, but we shall not consider this case, which would introduce additional technical complications. For simplicity of notation, many of the formulae that follow are written generically for the case $z = ix$; $x \in \mathbf{R}$, with the understanding that a suitable modification to the route is implied.

It will be useful to define the Fourier transform of the function $s(z)$ along the line L . We assume the branch cuts to be swept away from L , whence $s(z)$ is analytic and infinitely differentiable on $z \in L$. Let $L = a + \eta \mathbf{R}$, where a is a real number. By introducing the "conjugate" line $L' = i\eta^* \mathbf{R} = \eta' \mathbf{R}$ (hence $\eta\eta' = i$), we can define

$$s(z) \equiv \int_{L'} dx e^{xz} \hat{s}(x); \quad \hat{s}(x) = \int_L \frac{dz}{2\pi i} e^{-xz} s(z) \quad (z \in L, x \in L'). \quad (3.53a)$$

Since $s(z) \equiv \ln[f(z)/f(0)] \rightarrow -\frac{1}{2}z^2 + bz^\nu$, as $|z| \rightarrow \infty$, one observes that $\hat{s}(x)$ is actually a generalized function (i.e., a Schwartz distribution) [29]. Indeed, it is clear that apart from the term $-\frac{1}{2}\delta''(x)$, which contributes exactly at the origin, $\hat{s}(x)$ also has a power-law singularity $\propto |x|^{-\nu-1}$ near the origin. In the spirit of generalized functions the integrals of $\hat{s}(x)$ weighted by smooth test functions nevertheless exist. It was shown in detail in I how $\hat{s}(x)$ may be specifically and wholly represented in terms of the set of zeros of the holomorphic function $f(z)$. Some of the related mathematical aspects are further explored in Appendix B.

Our present definition differs slightly from the convention in I, where the constraint $s(0) = 0$ was forced by defining

$$s(z) \equiv \int_{-\infty}^{\infty} dx (e^{xz} - 1) \hat{s}(x); \quad \hat{s}(x) = \int_{-\infty}^{\infty} \frac{dy}{2\pi} e^{-ixy} s(iy). \quad (3.53b)$$

As was pointed out above, a small shift of x away from the real axis and z from the imaginary axis is now understood.

The definitions of Eqs. (3.53) can be used not only for general states $f(z)$ but also for the eigenstates $f^n(z)$ to define the functions $s^n(z)$ and $\tilde{s}_n(x)$. Because the odd eigenfunctions $f^{2m+1}(z)$ have a zero precisely at the origin, the corresponding $s^{2m+1}(z)$ can be thought to have an infinite constant term which, however, has no further consequences, since it is in fact only the derivative $s'(z)$ which is physically relevant, as is already evident from Eq. (2.23).

We now turn to the Bargmann amplitudes $\sigma(z)$ and $\tilde{\sigma}(z)$ which characterize the ECCM parametrization. We may use Eq. (2.28) in the form

$$\sigma(z) = \tilde{s}(d/dz) s(z) - \tilde{s}(d/dz) s(z)|_{z=0}, \quad (3.54)$$

together with the Fourier representation of $s(z)$ from Eqs. (3.53a)–(3.53b) to write $\sigma(z)$ in the form

$$\sigma(z) = \int_{-\infty}^{\infty} dx (e^{xz} - 1) \hat{\sigma}(x); \quad \hat{\sigma}(x) \equiv \tilde{s}(x) \hat{s}(x). \quad (3.55)$$

The asymptotic behaviour of $\tilde{s}(x)$, given in Eq. (3.49) for the anharmonic oscillator considered here, ensures that the integral expression for $\sigma(z)$ in Eq. (3.55) converges for all z , and hence that $\sigma(z)$ is an entire function. We can obtain another representation for the function $\sigma(z)$ by using the Fourier transform of $\tilde{s}$ rather than that of s in Eq. (3.54). We easily obtain for the general path L ,

$$\sigma^{(L)}(z) = \int_L \frac{d\zeta}{2\pi i} \tilde{s}_F(-i\zeta) [s(z + \zeta) - s(\zeta)]. \quad (3.56a)$$

For $z \in L$ we may perform a simple shift of variable in the first term in Eq. (3.56a), to obtain

$$\sigma^{(L)}(z) = \int_L \frac{d\zeta}{2\pi i} [\tilde{s}_F(iz - i\zeta) - \tilde{s}_F(-i\zeta)] s(\zeta), \quad z \in L. \quad (3.56b)$$

Due to the properties of the function $\tilde{s}_F(z)$ these expressions can be immediately analytically continued into the whole z plane. Equations (3.44)–(3.45) then show that $\sigma(z)$ is an entire function of order ν , just like the functions $\tilde{s}_F(z)$, $\phi(z)$, and $\chi(z)$.

We note that the function $\sigma(z)$ does not depend on any additive constant terms of $s(z)$. As the state $f(z)$ approaches an odd excited eigenstate, the function $s(z) = \ln[f(z)/f(0)]$ becomes singular due to $f(0) \rightarrow 0$, while $\sigma(z)$ remains regular. Another remark concerns the dependence of $\sigma^{(L)}(z)$ on the contour L . If, for example, L is moved across a particular zero z_m of $f(z)$ in such a way that z_m is initially to the right, and afterwards, to the left of L , with all other zeros staying on their original side of L , the function $\sigma^{(L)}(z)$ changes by the term

$$\Delta\sigma(z) = \int_{-z_m}^{z-z_m} du \tilde{s}_F(iu), \quad (3.57)$$

which is an entire function of order ν . Equation (3.57) is readily proved using Eqs. (3.56) and (B.2). This implies also a definite change in the set of coupled-cluster coefficients $\{\sigma_n\}$, which therefore in general cannot be completely uniquely specified. It is a simple matter to prove that the coefficients $\{\sigma_n\}$ are nevertheless independent of the precise position of L as long as it does not cross any zero of $f(z)$. This is done in Appendix B. Thus the set $\{\sigma_n\}$ is unique for each possible way in which the set of zeros can be divided by the line L . All of the other coupled-cluster coefficients, $\{s_n, \tilde{s}_n, \tilde{\sigma}_n\}$, are independent of L .

In spite of the fact that the set $\{\sigma_n\}$ need not be unique, the average value of an arbitrary operator, however, is invariant. These ECCM amplitudes therefore have attributes that are typical of *phase* functions, and the symmetry in question resembles a gauge symmetry.

Finally, the analytic properties of the ECCM function $\tilde{\sigma}(z) \equiv \ln \tilde{s}(z)$ depend upon the distribution of the zeros of the holomorphic function $\tilde{s}(z)$. Since for CC-representable states none of the zeros is located exactly at the origin, the conjugate line L' can always be determined such that $\tilde{\sigma}(z)$ is well defined and has a power-series expansion in z which is convergent within a finite radius. A solvable example is considered in Appendix C.

The definition of the coupled cluster representation for the states of the Hilbert space, as in Eqs. (2.9)–(2.10), leads to the introduction of an abstract manifold, the CCM phase space. By parametrizing the coupled-cluster operators one obtains a coordinate description of the manifold, which in this case is of infinite dimensionality. Manifolds are defined by the pairs (U_i, φ_i) , where $U_i \in M$ are the open sets and φ_i are homeomorphisms from U_i onto open subsets of the m -dimensional Euclidean space $\mathbf{R}^m$. In this framework the various ways to divide the zeros by the line L correspond to different inequivalent charts φ'_i by which the neighbourhood of the image point $p \in M$ of a given physical state (i.e., the pair $\langle \tilde{\Psi}|, |\Psi \rangle$) can be described on the manifold. A more detailed discussion of these aspects appears in paper III of the present series.

IV. EXPECTATION-VALUE FUNCTIONALS

IV.1. *The Generating Functional*

We now return to the computation of the average-value functional $\bar{O}$ of an arbitrary operator O in a general state which is not necessarily one of the eigenstates of the Hamiltonian, but which may otherwise be expressed as a sufficiently smooth linear combination of them so that it shares similar qualitative properties. That is, we require, for example, that the state is CC-representable in the sense of I, where it was pointed out that such states are dense in the Hilbert space. By expressing $\tilde{f}(z)$ in terms of its Fourier transform defined as in Eq. (3.21), we may rewrite Eq. (2.20) as

$$\begin{aligned}\bar{O} &= \int_{-\infty}^{\infty} \frac{dx}{2\pi} \tilde{f}_F(x) e^{ix(d/dz)} O\left(z, \frac{d}{dz}\right) f(z) \Big|_{z=0} \\ &= \int_{-\infty}^{\infty} \frac{dx}{2\pi} \tilde{f}_F(x) O\left(z+ix, \frac{d}{dz}\right) f(z+ix) \Big|_{z=0},\end{aligned}$$

and hence in the final CIM form,

$$\bar{O} = \int_{-\infty}^{\infty} \frac{dx}{2\pi} \tilde{f}_F(x) O\left(ix, -i \frac{d}{dx}\right) f(ix). \quad (4.1)$$

The NCCM form corresponding to Eq. (2.21) is now derived quite rigorously by using the analogue of Eq. (3.44), namely,

$$\tilde{s}_F(z) = \tilde{f}_F(z) f(iz), \quad (4.2)$$

to rewrite Eq. (4.1) as

$$\begin{aligned}\bar{O} &= \int_{-\infty}^{\infty} \frac{dx}{2\pi} \tilde{s}_F(x) [f(ix)]^{-1} O\left(ix, -i \frac{d}{dx}\right) f(ix) \\ &= \int_{-\infty}^{\infty} \frac{dx}{2\pi} \tilde{s}_F(x) e^{-s(ix)} O\left(ix, -i \frac{d}{dx}\right) e^{s(ix)} \\ &= \int_{-\infty}^{\infty} \frac{dx}{2\pi} \tilde{s}_F(x) O\left(ix, -i \frac{d}{dx} + s'(ix)\right).\end{aligned} \quad (4.3)$$

We note that Eq. (4.3) could also have been written immediately from Eq. (2.23). Nevertheless, the great advantage of proceeding via our results of Section III is that by so doing we have been able to prove that the integrals in Eq. (4.3) converge for practically all interesting operators $O(z, d/dz)$. These include all polynomials of the arguments z and d/dz and exponentials of the form $\exp(uz + v(d/dz))$. In this way we are able to justify such formal expressions as those for the NCCM parametrization in Eq. (2.9) and other such similar expressions in Section II, and the subsequent manipulations involving them.

As explained in Section III, it is important in the NCCM and ECCM to specify the integration path carefully. Starting from Eq. (4.1) in which the integrand is an analytic function in the whole complex x -plane and taking into account the asymptotic properties of the functions f and $\tilde{f}_F$, we have considerable freedom to choose the integration route. Referring to the discussion in Section III, we may adopt, for example,

$$\begin{aligned}\bar{O} &= \int_L \frac{d\zeta}{2\pi i} \tilde{f}_F(-i\zeta) O\left(\zeta, \frac{d}{d\zeta}\right) f(\zeta) \\ &= \int_L \frac{d\zeta}{2\pi i} \tilde{s}_F(-i\zeta) O\left(\zeta, \frac{d}{d\zeta} + s'(\zeta)\right).\end{aligned} \quad (4.4)$$

If the operator O is, for example, a finite-order polynomial of the canonical operators, we typically obtain terms of the form

$$\int_L \frac{d\zeta}{2\pi i} \tilde{s}_F(-i\zeta) \zeta^{k_0} s'(\zeta)^{k_1} s''(\zeta)^{k_2} s'''(\zeta)^{k_3} \dots,$$

where the exponents are $k_j \geq 0$. It is permissible to substitute each derivative of s by the integral expression obtained from Eq. (3.53), i.e., by using the functions $\hat{s}(x)$ instead. By changing the order of integrations we then recover the function $\tilde{s}$ and hence are also able to cast the terms in the ECCM form, using the definitions of Eq. (3.55) for the path L in question. However, this is a cumbersome way to calculate general averages.

We have also shown in I how an arbitrary expectation value $\bar{O}$ of an operator $O = O(a^\dagger, a)$ specified in normal-ordered form with respect to the operators a and $a^\dagger$, i.e., $O = :O:$, may be obtained in each of the three IC parametrizations from the generating functional

$$A(u, v) \equiv \langle \tilde{\Psi} | e^{ua^\dagger} e^{va} | \Psi \rangle, \quad (4.5)$$

as

$$\bar{O} = O(\partial_u, \partial_v) A(u, v)|_{u=v=0}, \quad (4.6)$$

where $\partial_u \equiv \partial/\partial u$, $\partial_v \equiv \partial/\partial v$. Furthermore, we have shown in I how $A(u, v)$ may be written in each ICM parametrization as an explicit functional of the corresponding Bargmann amplitudes which characterize the given parametrization. In the CIM we may write

$$A(u, v) \equiv A[u, v; f(ix), \tilde{f}_F(x)] = \int_{-\infty}^{\infty} \frac{dx}{2\pi} \tilde{f}_F(x) e^{ixu} f(v + ix), \quad (4.7a)$$

from which it is trivial to rederive Eq. (4.1) now for the case of normal-ordered operators. An equivalent expression is

$$A(u, v) \equiv A[u, v; f_F(x), \tilde{f}(ix)] = \int_{-\infty}^{\infty} \frac{dx}{2\pi} \tilde{f}(u + ix) e^{ixv} f_F(x). \quad (4.7b)$$

We have also shown in I that the alternative NCCM parametrization of $A(u, v)$ may be written in the form

$$\begin{aligned} A(u, v) &\equiv A[u, v; \hat{s}(x), \tilde{s}(x)] \\ &= \sum_{n=0}^{\infty} \frac{1}{n!} \prod_{i=1}^n \left[\int_{-\infty}^{\infty} dx_i (e^{x_i v} - 1) \hat{s}(x_i) \right] \tilde{s}(u + x_1 + \dots + x_n). \end{aligned} \quad (4.8)$$

Last, by making use of Eq. (3.55), we may also readily rewrite Eq. (4.8) in the ECCM form,

$$\begin{aligned}
 A(u, v) &\equiv A[u, v; \tilde{\sigma}(x), \tilde{\sigma}(x)] \\
 &= \sum_{n=0}^{\infty} \frac{1}{n!} \prod_{i=1}^n \left[\int_{-\infty}^{\infty} dx_i (e^{x_i v} - 1) \tilde{\sigma}(x_i) \right] \\
 &\quad \times \exp[\tilde{\sigma}(u + x_1 + \cdots + x_n) - \tilde{\sigma}(x_1) - \cdots - \tilde{\sigma}(x_n)]. \quad (4.9)
 \end{aligned}$$

The two CCM parametrizations of Eqs. (4.8) and (4.9) are particularly convenient forms for practical implementation. They are also easily rephrased for the case where the chart φ_i or line L (on which $s(z)$ is parametrized) is chosen differently.

IV.2. Example: Quartic Anharmonic Oscillator

As an example we shall consider the quartic anharmonic oscillator ($K=2$) and restrict ourselves to the case of the ECCM, where all the canonical amplitudes are sums of linked diagrams. The Hamiltonian can be easily written down in the explicit form,

$$\begin{aligned}
 H &= \frac{1}{2} \hat{p}^2 + \frac{1}{2} \hat{x}^2 + k \hat{x}^4 \\
 &= a^\dagger a + \frac{1}{2} + \frac{k}{4} (a^{\dagger 4} + 4a^\dagger a^3 + 6a^{\dagger 2} a^2 + 4a^\dagger a^3 + a^4 + 6a^{\dagger 2} + 12a^\dagger a + 6a^2 + 3). \quad (4.10)
 \end{aligned}$$

We apply the rule of Eq. (4.6) to the ECCM functional, Eq. (4.9), to derive the expectation value of the Hamiltonian,

$$\begin{aligned}
 \bar{H} &= \frac{1}{2} + \frac{k}{4} \left\{ 3 + 6\tilde{\sigma}''(0) + 6\tilde{\sigma}'(0)^2 + \tilde{\sigma}'''(0) + 4\tilde{\sigma}'''(0) \tilde{\sigma}'(0) + 3\tilde{\sigma}''(0)^2 + 6\tilde{\sigma}''(0) \tilde{\sigma}'(0)^2 \right. \\
 &\quad \left. + \tilde{\sigma}'(0)^4 \right\} + \int dx \left\{ \frac{k}{4} x^3 + k\tilde{\sigma}'(x) x^2 + \frac{3k}{2} [\tilde{\sigma}''(x) + \tilde{\sigma}'(x)^2 + 1] x \right. \\
 &\quad \left. + k[\tilde{\sigma}'''(x) + 3\tilde{\sigma}''(x) \tilde{\sigma}'(x) + \tilde{\sigma}'(x)^3 + 3\tilde{\sigma}'(x)] + \tilde{\sigma}'(x) \right\} x \tilde{\sigma}(x) \\
 &\quad + \iint dx_1 dx_2 \exp[\tilde{\sigma}(x_1 + x_2) - \tilde{\sigma}(x_1) - \tilde{\sigma}(x_2)] \times \left\{ kx_1^2 + \frac{3k}{4} x_1 x_2 \right. \\
 &\quad \left. + 3k\tilde{\sigma}'(x_1 + x_2) x_1 + \frac{3k}{2} [\tilde{\sigma}''(x_1 + x_2) + \tilde{\sigma}'(x_1 + x_2)^2 + 1] \right\} x_1 x_2 \tilde{\sigma}(x_1) \tilde{\sigma}(x_2)
 \end{aligned}$$

$$\begin{aligned}
 & + \iiint dx_1 dx_2 dx_3 \exp[\tilde{\sigma}(x_1 + x_2 + x_3) - \tilde{\sigma}(x_1) - \tilde{\sigma}(x_2) - \tilde{\sigma}(x_3)] \\
 & \times \left\{ \frac{3k}{2} x_1 + k\tilde{\sigma}'(x_1 + x_2 + x_3) \right\} x_1 x_2 x_3 \hat{\sigma}(x_1) \hat{\sigma}(x_2) \hat{\sigma}(x_3) \\
 & + \iiint\int dx_1 dx_2 dx_3 dx_4 \exp[\tilde{\sigma}(x_1 + x_2 + x_3 + x_4) - \tilde{\sigma}(x_1) \\
 & - \tilde{\sigma}(x_2) - \tilde{\sigma}(x_3) - \tilde{\sigma}(x_4)] \times \frac{k}{4} x_1 x_2 x_3 x_4 \hat{\sigma}(x_1) \hat{\sigma}(x_2) \hat{\sigma}(x_3) \hat{\sigma}(x_4). \quad (4.11)
 \end{aligned}$$

Our first remark concerning this expansion is that, under the conventions adopted for the amplitude functions, all of the integrals appearing in it converge and yield finite results for the various terms. This is true not only for the exact ground state but also for the case of an arbitrary CC-representable state. As discussed in I, such states are dense in the Hilbert space.

Second, we may analyze the expectation value in terms of the many-particle coupled-cluster coefficients $\{\sigma_m, \tilde{\sigma}_m\}$. Taking into account the definitions in Eqs. (2.10), we derive from Eq. (3.54) the following moment rules:

$$\sigma_n = \frac{1}{n!} \int_{-\infty}^{\infty} dx x^n \hat{\sigma}(x) \quad (n \geq 1). \quad (4.12a)$$

Similar results obviously also hold for the coefficients s_n of the NCCM ket-state amplitude,

$$s_n = \frac{1}{n!} \int_{-\infty}^{\infty} dx x^n \hat{s}(x) \quad (n \geq 1). \quad (4.12b)$$

By expanding the function $\tilde{\sigma}$ and its derivatives $\tilde{\sigma}^{(k)}$ as power series with coefficients $\tilde{\sigma}_m$, the remaining integrals yield factors of the amplitudes σ_n . The expectation value functional thus becomes a function of the n -particle amplitudes $\{\sigma_n, \tilde{\sigma}_n \mid n = 1, \dots, \infty\}$. We stress that the above form is a very economical way of correctly expressing or "renormalizing" these otherwise infinite (and often divergent) sums of fully linked diagrams. In Section VI we shall demonstrate that the expectation functional indeed sums only linked diagrams. (We note that for the general case allowing fermionic anticommuting coupled-cluster amplitudes, this was rigorously proven in Appendix A of Ref. [21].)

Third, the stationary states (and, in particular, the ground state) can be obtained by solving the nonlinear equations that express the stationarity of the energy functional. As given in I, the equations of motion are

$$i \frac{d\hat{\sigma}(x)}{dt} = \frac{\delta \bar{H}}{\delta \hat{\sigma}(x)}; \quad i \frac{d\hat{\sigma}(x)}{dt} = -\frac{\delta \bar{H}}{\delta \hat{\sigma}(x)}. \quad (4.13a)$$

At the stationary point we have

$$\frac{\delta \bar{H}}{\delta \hat{\sigma}(x)} = 0; \quad \frac{\delta \bar{H}}{\delta \tilde{\sigma}(x)} = 0. \quad (4.13b)$$

These equations are obviously complicated, and we will not explicitly write them down. Nevertheless, to get some flavour of such calculations we consider in Appendix C the solvable case of a squeezed harmonic oscillator, in both the NCCM and ECCM formalisms.

V. THE ICM STAR PRODUCT

V.1. Star Product Generation of Expectation Values

The expressions for average values can be generated by an alternative method which is based on the "ICM star product" first introduced in Ref. [20] and subsequently generalized to fermionic systems with anticommuting amplitudes [21]. This method is rather intrinsic and straightforward, and since it is purely algebraic, it may turn out to be useful in symbolic computing, for example. Again we only consider the case of the ECCM. The modifications required for the cases of the CIM and the NCCM are rather obvious.

The average value of the product of two operators, $\hat{A}$ and $\hat{B}$, can be given in the form

$$\overline{\hat{A}\hat{B}} = \bar{A} * \bar{B}, \quad (5.1)$$

where, as usual, the overlined symbols are average values and are thus certain functions or functionals of the canonical amplitudes $\{\sigma_n, \tilde{\sigma}_n\}$ or $\{\hat{\sigma}(x), \tilde{\sigma}(x)\}$. For simplicity of notation, in this section we equip operators with circumflexes and denote averages by plain letters, i.e., $\bar{A} \rightarrow A$, etc. With our present normalization conventions we obtain, by methods explained in detail in Ref. [20],

$$\begin{aligned} A * B = AB + \sum'_m \sum'_n \left\{ X_{m,n} \frac{\partial A}{\partial \sigma_m} \frac{\partial B}{\partial \sigma_n} + X_{m,\tilde{n}} \frac{\partial A}{\partial \sigma_m} \frac{\partial B}{\partial \tilde{\sigma}_n} \right. \\ \left. + X_{\tilde{m},n} \frac{\partial A}{\partial \tilde{\sigma}_m} \frac{\partial B}{\partial \sigma_n} + X_{\tilde{m},\tilde{n}} \frac{\partial A}{\partial \tilde{\sigma}_m} \frac{\partial B}{\partial \tilde{\sigma}_n} \right\}, \end{aligned} \quad (5.2)$$

where the primed summations go from one to infinity, and the coefficients are

$$X_{m,n} = \frac{(m+n)!}{m!n!} \sigma_{m+n} + \sum'_k \sum'_l \frac{(m+k)!(n+l)!}{m!n!} \sigma_{m+k} L_{k,l} \sigma_{l+n}, \quad (5.3a)$$

$$X_{m,\tilde{n}} = \frac{1}{m!} \delta_{m,n} + \sum'_k \frac{(m+k)!}{m!} \sigma_{m+k} L_{k,n}, \quad (5.3b)$$

$$X_{\tilde{m}, n} = \sum_k' \frac{(n+k)!}{n!} L_{m, k} \sigma_{k+n}, \quad (5.3c)$$

$$X_{\tilde{m}, \tilde{n}} = L_{m, n}. \quad (5.3d)$$

The summed indices in the above expressions are interpreted in the usual arithmetic sense without the associated redefinition of normalization as in Ref. [20].

The double-index amplitudes $L_{m, n} \equiv L_{m, n}[\tilde{\sigma}_l]$ are functions only of the variables $\tilde{\sigma}_l$ and are defined as follows [20]:

$$\begin{aligned} L_{m, n} &\equiv \frac{1}{m! n!} \langle 0 | \{ e^{\tilde{\Sigma}} a^{\dagger m} a^{+n} \}_{\mathcal{DL}} | 0 \rangle \\ &\equiv \frac{1}{m! n!} \sum_{l=0}^{\infty} \frac{1}{l!} \langle 0 | e^{\tilde{\Sigma}} a^{\dagger l} e^{-\tilde{\Sigma}} a^{+n} | 0 \rangle \langle 0 | a^l e^{-\tilde{\Sigma}} a^{+m} | 0 \rangle. \end{aligned} \quad (5.4)$$

Here the subscript $\mathcal{DL}$ denotes *double linking*, which requires each of the terms $\tilde{\Sigma}$ in the expansion of $\exp \tilde{\Sigma}$ to be linked to both the groups $a^{\dagger m}$ and a^{+n} . We define the generating function $L(x, y)$ for the coefficients and find

$$\begin{aligned} L(x, y) &\equiv \sum_{m=0}^{\infty} \sum_{n=0}^{\infty} x^m y^n L_{m, n} \\ &= \sum_{l=0}^{\infty} \frac{1}{l!} \langle 0 | e^{\tilde{\sigma}(a)} a^{\dagger l} e^{-\tilde{\sigma}(a)} e^{ya^{\dagger}} | 0 \rangle \langle 0 | a^l e^{-\tilde{\sigma}(a)} e^{xa^{\dagger}} | 0 \rangle \\ &= \sum_{l=0}^{\infty} \frac{1}{l!} \langle 0 | e^{\tilde{\sigma}(a+y)} a^{\dagger l} e^{-\tilde{\sigma}(a+y)} | 0 \rangle \langle 0 | (a+x)^l e^{-\tilde{\sigma}(a+x)} | 0 \rangle \\ &= \sum_{l=0}^{\infty} \frac{1}{l!} \langle 0 | e^{\tilde{\sigma}(a+y)} a^{\dagger l} | 0 \rangle e^{-\tilde{\sigma}(y) - \tilde{\sigma}(x)} x^l \\ &= \langle 0 | e^{\tilde{\sigma}(a+y)} e^{ya^{\dagger}} | 0 \rangle e^{-\tilde{\sigma}(y) - \tilde{\sigma}(x)}, \end{aligned} \quad (5.5)$$

from which we obtain

$$L(x, y) = e^{\tilde{\sigma}(x+y) - \tilde{\sigma}(x) - \tilde{\sigma}(y)}. \quad (5.6)$$

By calculating the partial derivative $\partial L(x, y)/\partial x$ from the definition on the first row of Eq. (5.5) and from Eq. (5.6) and equating equal powers of x and y on both sides it is straightforward to derive the recursion formula

$$L_{m, n} = \frac{1}{m} \sum_{k < m} \sum_{l < n} \frac{(m+n-k-l)!}{(m-1-k)! (n-l)!} \tilde{\sigma}_{m+n-k-l} L_{k, l}. \quad (5.7)$$

On the other hand, by taking the derivative with respect to $\tilde{\sigma}_k$ from the same two equations one easily derives the result

$$\frac{\partial L_{m,n}}{\partial \tilde{\sigma}_k} = \sum_{l=1}^{k-1} \frac{k!}{l!(k-l)!} L_{m-l, n-k+l}. \quad (5.8)$$

Special cases of the above formulae are: $L(x, 0) = 1$; $L_{n,0} = \delta_{n,0}$; $L_{1,n} = (n+1) \tilde{\sigma}_{n+1}$ (for $n \geq 1$); and $\partial L_{m,n} / \partial \tilde{\sigma}_2 = 2L_{m-1, n-1}$.

For the product of more than two factors, each of which is an expectation value of some operator, the star product is associative [20], $A * (B * C) = (A * B) * C$. An arbitrary operator can be obtained, for example, from terms that are products of the primitive canonical operators $a, a^\dagger$. Their averages are clearly,

$$\overline{a^\dagger} = \tilde{\sigma}_1; \quad \bar{a} = \sigma_1. \quad (5.9)$$

Higher-order averages are thus

$$\overline{a^\dagger a^\dagger \cdots a^\dagger a \cdots a} = \tilde{\sigma}_1 * \tilde{\sigma}_1 * \cdots * \tilde{\sigma}_1 * \sigma_1 * \cdots * \sigma_1. \quad (5.10)$$

There is actually no need to restrict to normal order, because the star product is defined for arbitrary operators. To develop such products systematically, it is necessary to calculate the products $\tilde{\sigma}_1 * A$ and $A * \sigma_1$ for general operators A . The results can be cast into the forms

$$\tilde{\sigma}_1 * A = \left[\tilde{\sigma}_1 + \sum'_m \left(J_m^1 \frac{\partial}{\partial \sigma_m} + K_m^1 \frac{\partial}{\partial \tilde{\sigma}_m} \right) \right] A, \quad (5.11a)$$

$$A * \sigma_1 = \left[\sigma_1 + \sum'_m \left(J_m^2 \frac{\partial}{\partial \sigma_m} + K_m^2 \frac{\partial}{\partial \tilde{\sigma}_m} \right) \right] A, \quad (5.11b)$$

where the coefficient functions are

$$J_m^1 = \sum'_k (k+1) \frac{(m+k)!}{m!} \tilde{\sigma}_{k+1} \sigma_{k+m}, \quad (5.12a)$$

$$K_m^1 = (m+1) \tilde{\sigma}_{m+1}, \quad (5.12b)$$

$$J_m^2 = (m+1) \sigma_{m+1} + \sum'_k \sum'_l \frac{(m+k)! (l+1)!}{m!} \sigma_{m+k} L_{k,l} \sigma_{l+1}, \quad (5.12c)$$

$$K_m^2 = \sum'_k (k+1)! L_{m,k} \sigma_{k+1}. \quad (5.12d)$$

The simplest applications of these formulae are the second-order products

$$\overline{a^{\dagger 2}} = \tilde{\sigma}_1 * \tilde{\sigma}_1 = \tilde{\sigma}_1 \tilde{\sigma}_1 + K_1^1 = \tilde{\sigma}_1^2 + 2\tilde{\sigma}_2, \quad (5.13a)$$

$$\overline{a^{\dagger} a} = \tilde{\sigma}_1 * \sigma_1 = \tilde{\sigma}_1 \sigma_1 + J_1^1 = \sum_k' k k! \tilde{\sigma}_k \sigma_k, \quad (5.13b)$$

$$\overline{a^2} = \sigma_1 * \sigma_1 = \sigma_1 \sigma_1 + J_1^2 = 2\sigma_2 + \sum_k' \sum_l' k! l! \sigma_k \sigma_l L_{k-1, l-1}. \quad (5.13c)$$

We may also formulate these rules using the canonical functions $\hat{\sigma}(x)$, $\tilde{\sigma}(x)$ and functional derivatives with respect to them. An average-value functional is then $A[\hat{\sigma}(x), \tilde{\sigma}(x)]$. For that purpose we calculate the following rules for the partial derivatives:

$$\frac{\partial A}{\partial \sigma_n} = \frac{d^n}{dx^n} \frac{\delta A}{\delta \tilde{\sigma}(x)} \Big|_{x=0}; \quad \frac{\partial A}{\partial \tilde{\sigma}_n} = \int dx x^n \frac{\delta A}{\delta \tilde{\sigma}(x)} \quad (n \geq 1) \quad (5.14a)$$

$$\frac{\partial A}{\partial \hat{\sigma}(x)} = \sum_n' \frac{x^n}{n!} \frac{\partial A}{\partial \sigma_n}; \quad \frac{\delta A}{\delta \tilde{\sigma}(x)} = \sum_n' \frac{(-1)^n}{n!} \delta^{(n)}(x) \frac{\partial A}{\partial \tilde{\sigma}_n}. \quad (5.14b)$$

From the coefficients of Eq. (5.12) we build the functions

$$J^{1,2}(z) = \sum_n' J_n^{1,2} z^n; \quad K^{1,2}(z) = \sum_n' K_n^{1,2} z^n. \quad (5.15)$$

Using the representation of Eq. (4.12a) for each amplitude σ_k appearing in Eqs. (5.12), we use rather straightforward algebra to calculate these functions and find the results,

$$J^1(z) = \int dx (e^{xz} - 1) [\tilde{\sigma}'(x) - \tilde{\sigma}_1] \tilde{\sigma}(x), \quad (5.16a)$$

$$J^2(z) = \int dx (e^{xz} - 1) \tilde{\sigma}(x) \left\{ x + \int dy [L(x, y) - 1] y \tilde{\sigma}(y) \right\}, \quad (5.16b)$$

$$K^1(z) = \tilde{\sigma}'(z) - \tilde{\sigma}_1, \quad (5.16c)$$

$$K^2(z) = \int dx [L(x, z) - 1] x \tilde{\sigma}(x). \quad (5.16d)$$

From Eqs. (5.14)–(5.15) one finds that

$$\sum_n' J_n^1 \frac{\partial A}{\partial \sigma_n} = J^1 \left(\frac{d}{dz} \right) \frac{\delta A}{\delta \tilde{\sigma}(z)} \Big|_{z=0}; \quad \sum_n' K_n^1 \frac{\partial A}{\partial \tilde{\sigma}_n} = \int dx K^1(x) \frac{\delta A}{\delta \tilde{\sigma}(x)}. \quad (5.17)$$

Using the same rules also for the remaining summations in Eqs. (5.11) and substituting the explicit forms of Eqs. (5.16) we find the final results,

$$\overline{a^{\dagger} * A} = \tilde{\sigma}_1 A + \int dx [\tilde{\sigma}'(x) - \tilde{\sigma}_1] \left[\frac{\delta A}{\delta \tilde{\sigma}(x)} + \tilde{\sigma}(x) \frac{\delta A}{\delta \tilde{\sigma}(x)} \right], \quad (5.18a)$$

$$A * \bar{a} = A \sigma_1 + \int dx [\tau_1(x) - \sigma_1] \frac{\delta A}{\delta \tilde{\sigma}(x)} + \int dx [x + \tau_1(x) - \sigma_1] \tilde{\sigma}(x) \frac{\delta A}{\delta \tilde{\sigma}(x)}, \quad (5.18b)$$

where we have denoted

$$\tau_1(x) \equiv \int dy L(x, y) y \hat{\sigma}(y). \quad (5.19)$$

We note that $\tau_1(0) = \sigma_1$. Actually, if Eqs. (5.18) are iterated several times, we need to substitute $\tilde{\sigma}_1 \rightarrow \tilde{\sigma}'(0)$ and $\sigma_1 \rightarrow \int dx x \hat{\sigma}(x)$, whence the right-hand sides of Eqs. (5.18) will be represented throughout in terms of the functions $\hat{\sigma}(x)$ and $\tilde{\sigma}(x)$.

The above results simplify slightly if we assume the function $\tilde{\sigma}(z)$ to be unrestricted by the requirement $\tilde{\sigma}(0) = 0$. This is perfectly legitimate because the value $\tilde{\sigma}(0)$ is a constant of motion, just as is the NCCM amplitude $\tilde{s}(0)$. From the equations of motion, Eqs. (4.13a), we find

$$i\dot{\tilde{\sigma}}(0) = -\frac{\delta \bar{H}}{\delta \tilde{\sigma}(0)} = 0, \quad (5.20)$$

where the last equality is obvious on the basis of the expression for the generating functional (4.9) for the average values. Therefore we can assume $\tilde{\sigma}(0)$ to be completely unrestricted and fix its value only at the end of the calculation. In this case the expressions for certain average values, such as the purely creative or constant terms in Eq. (4.11), must be supplied with the appropriate explicit factor $\exp \tilde{\sigma}(0)$. Assuming that this is taken care of, it is a straightforward matter to show that the identity

$$\int dx \left[\frac{\delta A}{\delta \tilde{\sigma}(x)} + \hat{\sigma}(x) \frac{\delta A}{\delta \hat{\sigma}(x)} \right] = A \quad (5.21)$$

holds for any operator. This is a consequence of the symmetry

$$A[e^{\lambda} \hat{\sigma}(x), \tilde{\sigma}(x) + \lambda] = e^{\lambda} A[\hat{\sigma}(x), \tilde{\sigma}(x)], \quad (5.22)$$

which can be readily proven using the generating functional, Eq. (4.9). Using the identity (5.21) we therefore obtain the alternative simpler forms,

$$\bar{a}^\dagger * A = \int dx \tilde{\sigma}'(x) \left[\frac{\delta A}{\delta \tilde{\sigma}(x)} + \hat{\sigma}(x) \frac{\delta A}{\delta \hat{\sigma}(x)} \right], \quad (5.23a)$$

$$A * \bar{a} = \int dx \tau_1(x) \frac{\delta A}{\delta \tilde{\sigma}(x)} + \int dx [x + \tau_1(x)] \hat{\sigma}(x) \frac{\delta A}{\delta \hat{\sigma}(x)}. \quad (5.23b)$$

The general case of arbitrary operators, Eqs. (5.2)–(5.3), can be treated in the same way. We omit the intermediate steps of the derivation and give only the final result,

$$\begin{aligned}
 A * B = AB &+ \iint dx dy \frac{\delta A}{\delta \tilde{\sigma}(x)} \frac{\delta B}{\delta \tilde{\sigma}(y)} [L(x, y) - 1] \\
 &+ \iint dx dy \frac{\delta A}{\delta \tilde{\sigma}(x)} \frac{\delta B}{\delta \tilde{\sigma}(y)} \tilde{\sigma}(y) [L(x, y) - 1] \\
 &+ \iint dx dy \frac{\delta A}{\delta \tilde{\sigma}(x)} \frac{\delta B}{\delta \tilde{\sigma}(y)} \{ \tilde{\sigma}(x) [L(x, y) - 1] + \delta(x - y) \} \\
 &+ \iint dx dy \frac{\delta A}{\delta \tilde{\sigma}(x)} \frac{\delta B}{\delta \tilde{\sigma}(y)} \{ \tilde{\sigma}(x) \tilde{\sigma}(y) [L(x, y) - 1] + \tilde{\sigma}(x) \delta(x - y) \}. \quad (5.24)
 \end{aligned}$$

The star product can be used to introduce the Poisson bracket in accordance with Ref. [20]. The definition is

$$i\{A, B\} \equiv \langle [\hat{A}, \hat{B}] \rangle, \quad (5.25)$$

and if we apply the formulae given above for the star product we can derive the following results for the ECCM,

$$\begin{aligned}
 i\{A, B\} &\equiv A * B - B * A \\
 &= \sum_n \frac{1}{n!} \left[\frac{\partial A}{\partial \sigma_n} \frac{\partial B}{\partial \tilde{\sigma}_n} - \frac{\partial B}{\partial \sigma_n} \frac{\partial A}{\partial \tilde{\sigma}_n} \right] \\
 &= \int dx \left[\frac{\delta A}{\delta \tilde{\sigma}(x)} \frac{\delta B}{\delta \tilde{\sigma}(x)} - \frac{\delta B}{\delta \tilde{\sigma}(x)} \frac{\delta A}{\delta \tilde{\sigma}(x)} \right]. \quad (5.26)
 \end{aligned}$$

Using the Poisson bracket one can write the equations of motion for arbitrary operators in a unified form,

$$i \frac{dA}{dt} = i \frac{\partial A}{\partial t} + i\{A, H\} = i \frac{\partial A}{\partial t} + (A * H - H * A), \quad (5.27)$$

where the partial time derivative is taken with respect to the possible explicit time dependence of the operator. Another particular result which facilitates the application of these formulae is

$$i\{\tilde{\sigma}(x), \tilde{\sigma}(y)\} \equiv \tilde{\sigma}(x) * \tilde{\sigma}(y) - \tilde{\sigma}(y) * \tilde{\sigma}(x) = \delta(x - y). \quad (5.28)$$

The functions $(\tilde{\sigma}(x), \tilde{\sigma}(x))$ are thus canonically conjugated fields with regard to the classical Poisson bracket. Similar structures can also be introduced in the NCCM and CIM.

Equations (5.2) or (5.24) show that the ICM (in this case ECCM) star multiplication mixes ordinary multiplication with the computation of the first-order differentials of the functions on the ECCM manifold. In particular, the coefficients

X in Eq. (5.2) may be interpreted as components of a certain tensor X of type $(2, 0)$, by means of which we can express the star product also in the coordinate-free form,

$$A * B \equiv AB + X(dA, dB) = AB + \sum_{\mu\nu} X^{\mu\nu} \frac{\partial A}{\partial x^\mu} \frac{\partial B}{\partial x^\nu}, \quad (5.29)$$

where d is the exterior derivative and dA, dB are one-forms, and $X^{sv} \equiv X(dx^\mu, dx^\nu)$ are the components of the tensor in the basis of the cotangent space. The connection of the present notation to that in Eq. (5.2) is obvious. The tensor X is defined once and for all for the manifold, and it is related to its differential and "combinatorial" structure. These observations, together with the fact that the whole coupled-cluster manifold and the vector fields themselves can thus be constructed by successive multiplications, relate the star product to the differential topology of these manifolds and to the process of quantization of a classical theory.

The expressions of this subsection are useful, for example, due to the fact that by using them the average values are explicitly built out of the ECCM canonical amplitudes, namely, either $\{\sigma_n, \bar{\sigma}_n\}$ or $\{\hat{\sigma}(x), \bar{\sigma}(x)\}$. This is, of course, valuable *per se*, but it also has practical computational consequences. For example, in earlier numerical works (such as in Refs. [30, 31]) difficulties have arisen due partly to the practical necessity of using the NCCM amplitudes $\{s_n, \bar{s}_n\}$ as intermediate steps in constructing the energy functional, which in an ECCM computation forces one to make transitions between the NCCM and ECCM amplitude sets. Some of these changes of variables are numerically rather delicate and introduce unnecessary rounding errors which reduce the accuracy in high-order truncations. Such practical problems may be easier to avoid by the present more direct computational methods.

V.2. Criteria for Expectation Value Functionals and Associativity of the Star Product

We may enquire whether a given functional $O[\hat{\sigma}, \bar{\sigma}]$ of the functions $\hat{\sigma}(x), \bar{\sigma}(x)$ actually represents the average value of some operator. In this subsection we formulate the necessary and sufficient conditions for this to be case and point out the connection of this problem to the question of the associativity of the ICM star product.

Obviously the functional $O[\hat{\sigma}, \bar{\sigma}]$ is an average value, if it can be reverted to the original CIM average-value form of Eq. (4.1) by performing the nonlinear CCM transformations backwards, from $\{\hat{\sigma}(x), \bar{\sigma}(x)\}$ to $\{f(ix), \tilde{f}_F(x)\}$. Since the CIM expression (4.1) is linear in both f and $\tilde{f}_F$, we obtain the conditions,

$$\int dx \frac{\delta O}{\delta f(ix)} f(ix) = 0, \quad (5.30a)$$

$$\int dx \frac{\delta O}{\delta \tilde{f}_F(x)} \tilde{f}_F(x) = 0, \quad (5.30b)$$

which are characteristic for homogeneous functions of first order. In these equations

we consider the variations of $f(ix)$ and $\tilde{f}_F(x)$ to be unrestricted by normalization requirements. Therefore we neither impose the condition $\tilde{s}(0)=1$, $\tilde{\sigma}(0)=0$, nor $s(0)=0$. Equations (5.30) must now be given in terms of the free variables $\{\hat{\sigma}(x), \tilde{\sigma}(x)\}$. Using the definitions $f(ix)=\exp s(ix)$, $\tilde{s}(x)=\exp \tilde{\sigma}(x)$ together with those in Eqs. (3.43), (3.53a), (3.55), and (4.2), we can cast the rules for the partial functional derivatives in the following convenient forms:

$$D_u \equiv \int dx e^{ixu} f(ix) \frac{\delta}{\delta f(ix)} \\ = e^{\tilde{\sigma}(u)} \left\{ \frac{\delta}{\delta \tilde{\sigma}(u)} + \int dy L(u, y) \left[\frac{\delta}{\delta \tilde{\sigma}(y)} + \tilde{\sigma}(y) \frac{\delta}{\delta \tilde{\sigma}(y)} \right] \right\}, \quad (5.31a)$$

$$\tilde{D}_u \equiv \int dx e^{-ixu} \frac{1}{f(ix)} \frac{\delta}{\delta \tilde{f}_F(x)} \\ = e^{-\tilde{\sigma}(u)} \left[\frac{\delta}{\delta \tilde{\sigma}(u)} + \tilde{\sigma}(u) \frac{\delta}{\delta \tilde{\sigma}(u)} \right]. \quad (5.31b)$$

Equation (5.30b) now leads to the condition

$$\int du e^{\tilde{\sigma}(u)} \tilde{D}_u O = O, \quad (5.32a)$$

which immediately yields the earlier derived result of Eq. (5.21). Equation (5.30a) leads to a condition, which, by taking into account the just-derived result of Eq. (5.21), can be simplified to the form

$$\frac{\partial O}{\partial \tilde{\sigma}(0)} = 0. \quad (5.32b)$$

These two conditions can also be formulated in terms of the multi-particle coupled-cluster amplitudes $\{\sigma_n, \tilde{\sigma}_n\}$. Since we have given up the requirement of normalization, we now allow the amplitudes σ_0 and $\tilde{\sigma}_0$ to be nonzero and to be defined by Eq. (4.12a) for $n=0$ and $\tilde{\sigma}_0 = \tilde{\sigma}(0)$, respectively. The transition between the two sets of variables is still given by Eqs. (5.14), but with the terms $n=0$ allowed. It is then quite straightforward to show that the conditions of Eqs. (5.32) combine to the following results:

$$\frac{\partial O}{\partial \tilde{\sigma}_0} + \sum_{n=1}^{\infty} \sigma_n \frac{\partial O}{\partial \sigma_n} = O; \quad \frac{\partial O}{\partial \sigma_0} = 0. \quad (5.33)$$

An observable thus cannot depend on the newly allowed amplitude σ_0 , and under the transformation $\tilde{\sigma}_0 \rightarrow \tilde{\sigma}_0 + \lambda$, $\sigma_n \rightarrow e^{\lambda} \sigma_n$ ($n \geq 1$) it must change as $O \rightarrow e^{\lambda} O$ (cf., Eq. (5.22)).

On the other hand, if normalization is assumed throughout, whence $\sigma_0 = \tilde{\sigma}_0 = 0$

in accordance with the definitions of Section II, it is easy to show that Eqs. (5.33) amount to nought, in the sense that they provide no new conditions.

Although the above two conditions are necessary requirements for the functional O to represent an average value, they are not sufficient. Indeed, even if they are satisfied, the second functional derivatives of O with respect to $f(ix)$ or $\tilde{f}_F(x)$ may be nonzero. We can exemplify this by considering the case of 1 + 1 real variables $x, \tilde{x}$. Assuming that the function $w(x, \tilde{x})$ is a linear homogeneous function of both variables, it must satisfy the requirements

$$x \frac{\partial w}{\partial x} = \tilde{x} \frac{\partial w}{\partial \tilde{x}} = w.$$

However, the general solution of these equations is still of the form

$$w = Ax\tilde{x} + Bx|\tilde{x}| + C|x|\tilde{x} + D|x\tilde{x}|.$$

The function w is therefore proportional to $x\tilde{x}$ in every quadrant of the $x, \tilde{x}$ -plane, but with different coefficients in each of them. The nodal surfaces separate the phase space into disjoint sectors with independent solutions. Thus the function w is not globally linear in both variables. The minimum ingredient to guarantee global linearity is to require that, in addition, the second derivatives satisfy

$$\frac{\partial^2 w}{\partial x^2} = \frac{\partial^2 w}{\partial \tilde{x}^2} = 0$$

at the nodal surfaces. However, it is difficult to restrict this requirement only to nodal surfaces. Instead it is easier to demand that this condition be satisfied everywhere. Alternative additional requirements may be formulated if it is known or required that the function w has some specific analyticity properties for complex arguments.

For functions of several variables the above results are still obvious. In the present case we have complex-valued functionals of a continuous set of variables, and the arguments do not carry through very easily. Nevertheless, it is obvious that the conditions (5.30) must be augmented by additional requirements and that for that purpose we can use the conditions

$$\frac{\delta^2 O}{\delta f(ix) \delta f(iy)} = 0, \quad (5.34a)$$

$$\frac{\delta^2 O}{\delta \tilde{f}_F(x) \delta \tilde{f}_F(y)} = 0. \quad (5.34b)$$

In fact, these conditions guarantee that O is a functional which is at most of first order both in f and in $\tilde{f}_F$, and the requirements of Eqs. (5.30) further eliminate the possibility of inhomogeneous (zero order) terms.

By simple manipulations the above conditions can be cast in the equivalent forms,

$$(D_u D_v - D_{u+v}) O = 0, \quad (5.35a)$$

$$\tilde{D}_u \tilde{D}_v O = 0. \quad (5.35b)$$

The latter, which is simpler, yields the consistency requirement

$$\begin{aligned} \frac{\delta^2 O}{\delta \tilde{\sigma}(u) \delta \tilde{\sigma}(v)} + \hat{\sigma}(u) \frac{\delta^2 O}{\delta \hat{\sigma}(u) \delta \tilde{\sigma}(v)} + \hat{\sigma}(v) \frac{\delta^2 O}{\delta \tilde{\sigma}(u) \delta \hat{\sigma}(v)} \\ + \hat{\sigma}(u) \hat{\sigma}(v) \frac{\delta^2 O}{\delta \hat{\sigma}(u) \delta \hat{\sigma}(v)} = \delta(u-v) \frac{\delta O}{\delta \tilde{\sigma}(u)}. \end{aligned} \quad (5.36a)$$

In terms of the coupled-cluster amplitudes $\{\sigma_n, \tilde{\sigma}_n \mid n \geq 1\}$ Eq. (5.36a) may be equivalently written as

$$\begin{aligned} \frac{\partial^2 O}{\partial \tilde{\sigma}_i \partial \tilde{\sigma}_j} + \sum_k' \frac{(i+k)!}{k!} \sigma_{i+k} \frac{\partial^2 O}{\partial \sigma_k \partial \tilde{\sigma}_j} + \sum_l' \frac{(j+l)!}{l!} \sigma_{j+l} \frac{\partial^2 O}{\partial \sigma_l \partial \tilde{\sigma}_i} \\ + \sum_k' \sum_l' \frac{(i+k)! (j+l)!}{k! l!} \sigma_{i+k} \sigma_{j+l} \frac{\partial^2 O}{\partial \sigma_k \partial \sigma_l} = \frac{\partial O}{\partial \tilde{\sigma}_{i+j}} \quad (i, j \geq 1). \end{aligned} \quad (5.36b)$$

This equation (with the standard normalized index conventions) was derived already in Ref. [20] for the general case.

The other equation, (5.35a), yields a condition which can be simplified by the result of Eq. (5.36a) to the final form,

$$\begin{aligned} \frac{\delta^2 O}{\delta \hat{\sigma}(u) \delta \hat{\sigma}(v)} + \int dx L(u, x) \left[\frac{\delta^2 O}{\delta \tilde{\sigma}(x) \delta \hat{\sigma}(v)} + \hat{\sigma}(x) \frac{\delta^2 O}{\delta \hat{\sigma}(x) \delta \hat{\sigma}(v)} \right] \\ + \int dx L(v, x) \left[\frac{\delta^2 O}{\delta \tilde{\sigma}(x) \delta \hat{\sigma}(u)} + \hat{\sigma}(x) \frac{\delta^2 O}{\delta \hat{\sigma}(x) \delta \hat{\sigma}(u)} \right] \\ = L(u, v) \left[\frac{\delta O}{\delta \hat{\sigma}(u+v)} - \frac{\delta O}{\delta \hat{\sigma}(u)} - \frac{\delta O}{\delta \hat{\sigma}(v)} \right]. \end{aligned} \quad (5.37a)$$

In terms of the amplitudes $\{\sigma_n, \tilde{\sigma}_n \mid n \geq 1\}$ this condition is equivalently written as

$$\begin{aligned} \frac{1}{i! j!} \frac{\partial^2 O}{\partial \sigma_i \partial \sigma_j} + \sum_k' \frac{1}{j!} L_{i,k} \frac{\partial^2 O}{\partial \tilde{\sigma}_k \partial \sigma_j} + \sum_l' \frac{1}{i!} L_{j,l} \frac{\partial^2 O}{\partial \tilde{\sigma}_l \partial \sigma_i} \\ + \sum_k' \sum_l' \frac{(k+l)!}{j! k!} L_{i,l} \sigma_{k+l} \frac{\partial^2 O}{\partial \sigma_k \partial \sigma_j} + \sum_k' \sum_l' \frac{(k+l)!}{i! l!} L_{j,k} \sigma_{k+l} \frac{\partial^2 O}{\partial \sigma_l \partial \sigma_i} \\ = \sum_{k=2}^{\infty} \frac{1}{k!} \frac{\partial L_{i,j}}{\partial \tilde{\sigma}_k} \frac{\partial O}{\partial \sigma_k}, \quad (i, j \geq 1). \end{aligned} \quad (5.37b)$$

To prove Eqs. (5.36b) and (5.37b) it is easiest to proceed as explained below Eqs. (5.32), by first assuming the non-normalized convention and thus allowing nonzero σ_0 and $\tilde{\sigma}_0$. The partial derivatives with respect to σ_0 and $\tilde{\sigma}_0$ are subsequently eliminated using Eqs. (5.33). The final result is then valid also for the normalized convention.

An alternative procedure is to use, throughout, the normalized convention for the many-body amplitudes $\{\sigma_n, \tilde{\sigma}_n\}$. In this case we must define

$$\sigma_n = \frac{1}{n!} \int_{-\infty}^{\infty} dx x^n \exp[\tilde{\sigma}(x) - \tilde{\sigma}(0)] \hat{s}(x),$$

instead of Eq. (4.12a). The functional derivatives with respect to $\hat{\sigma}(x)$, $\tilde{\sigma}(x)$ are now

$$\begin{aligned} \frac{\delta}{\delta \hat{\sigma}(x)} &= e^{-\tilde{\sigma}_0} \sum_{n=0}^{\infty} \frac{x^n}{n!} \frac{\partial}{\partial \sigma_n}; \\ \frac{\delta}{\delta \tilde{\sigma}(x)} &= \sum_{n=0}^{\infty} \frac{(-1)^n}{n!} \delta^{(n)}(x) \frac{\partial}{\partial \tilde{\sigma}_n} - \delta(x) \sum_{n=0}^{\infty} \sigma_n \frac{\partial}{\partial \sigma_n}. \end{aligned}$$

We also must take note of the fact that the functional O appearing in Eqs. (5.30), (5.32), (5.35), (5.36a), and (5.37a) is the non-normalized average-value functional. If it is substituted by the expression $\exp(\tilde{\sigma}_0)O$, the new O is the normalized average-value functional. It is then quite straightforward to show that Eqs. (5.32) lead to the conditions $\partial O / \partial \sigma_0 = \partial O / \partial \tilde{\sigma}_0 = 0$ for this normalized O , showing that it cannot depend on σ_0 or $\tilde{\sigma}_0$. Eqs. (5.36b) and (5.37b) can be derived in a similar way, with the interpretation that both O and the many-body amplitudes $\{\sigma_n, \tilde{\sigma}_n | n \geq 1\}$ appearing in them correspond to the convention of manifest normalization.

On the other hand, the forms of Eqs. (5.36b) and (5.37b) are inferior to the forms (5.36a) and (5.37a) because the discrete summations over the labels $\{n\}$ almost invariably diverge (some examples were considered in I). The corresponding versions of Eqs. (5.36a) and (5.37a) are given in terms of the properly renormalized convergent sums of those divergent expansions.

The consistency relations derived in this subsection are vital for guaranteeing the associativity of the star product for observables. Indeed, for general functionals, $(A * B) * C \neq A * (B * C)$. If the rule of Eq. (5.24) is applied repeatedly to compute $(A * B) * C$, there will appear second-order functional derivatives of A , while such terms do not appear in the expression $A * (B * C)$, which, on the other hand, contains second-order functional derivatives of C which are absent from the first expression. If A , B , and C are observables, Eqs. (5.36) and (5.37) can now be used to simplify these expressions to the extent that neither of them contains second-order functional derivatives of A or C , and, furthermore, so that they agree.

The space $\mathcal{F}^c(M)$ of functions satisfying the consistency requirements of Eqs. (5.21), (5.32b), (5.36), and (5.37) is a subspace of the space $\mathcal{F}(M)$ of all (smooth) functions on the ECCM manifold M . It is true that if A and B satisfy the

above consistency relations so does their star product $A * B$. The star product therefore introduces a ring structure in the space $\mathcal{F}^c(M)$. With respect to ordinary multiplication this subspace is not closed. That is, even if $A \in \mathcal{F}^c(M)$ and $B \in \mathcal{F}^c(M)$, the product $AB \notin \mathcal{F}^c(M)$.

The functions in $\mathcal{F}^c(M)$ form an associative algebra under the star product. Thus, if $A, B, C \in \mathcal{F}^c(M) \subset \mathcal{F}(M)$, then $(A * B) * C = A * (B * C)$. The space $\mathcal{F}^c(M)$ can be identified with the set of observables of the ECCM theory. The totality of all functions in $\mathcal{F}(M)$ forms an algebra which is neither commutative nor associative under the CCM star product. We shall speak more in III on the manifold aspects of the ICM phase spaces. Nevertheless, it goes without saying that in our case the manifold M is an infinite-dimensional functional phase space (spanned by the coordinate functions or generalized functions such as $\{\hat{\sigma}(x), \tilde{\sigma}(x)\}$ in the ECCM), and $\mathcal{F}(M)$ is the space of functionals rather than functions.

We note, in particular, that the canonical amplitudes $\{\hat{\sigma}(x), \tilde{\sigma}(x)\}$ themselves do not form an associative algebra. For example, we find

$$(\tilde{\sigma}(x) * \tilde{\sigma}(y)) * \tilde{\sigma}(z) - \tilde{\sigma}(x) * (\tilde{\sigma}(y) * \tilde{\sigma}(z)) = [L(x, y) - L(y, z)][1 - L(x, z)] \neq 0.$$

In this respect these amplitudes are precisely comparable to the Schrödinger wave function $\psi(x)$, which is also not an average value of any operator. However, they obviously have important physical meaning as quantities that have been derived or abstracted from some more observation-related information. Although they play the role of the generalized canonical coordinates and momenta in the ICM phase spaces, it may seem that these amplitudes are less physical than the corresponding quantities in classical physics, where, by definition, all functions are usually claimed to be observable (with the exception of classical gauge fields which are needed in the canonical formulation of field theories but are not directly measurable). We may be tempted to call them "hidden variables" in the usual meaning. If this is reasonable to do, the criteria of this subsection provide a possible precise mathematical definition for the concept of a "hidden" variable, as opposed to the "physical" variables.

The canonical coordinates $x = (\tilde{\sigma}_1 + \sigma_1)/\sqrt{2}$, $p = i(\tilde{\sigma}_1 - \sigma_1)/\sqrt{2}$ of the original Hamiltonian remain, nevertheless, observables in the sense of the present definition. It is therefore legal to consider their star products of arbitrary order and arrangement, such as $x * x * p * x * p$. The process of quantization thus corresponds to the mapping

$$H(x, p) \mapsto H(*x, *p), \quad (5.38)$$

where the ordinary products are replaced by the star products, and the dimensionality of the manifold is increased according to a definite scheme. The result is naturally not completely unique due to the well-known freedom in the ordering of the factors and due to the discrete multiplicity of the representative point in the ECCM phase space, as discussed in Sections III, IV.

Equations (5.21), (5.32b), (5.33), (5.36), and (5.37) are conceptually related to

the Ward (or Slavnov–Taylor) identities in the theory of Green’s functions, in the sense that both sets are concerned with the consistency of the diagrammatic structure.

V.3. Comparison with Deformation Theory and the Moyal Star Product

There is a long tradition in quantum mechanics of developing alternative ways for the process of quantization, in addition to the usual Hilbert space method. The most notable example is the path integral method of Feynman. A second autonomous example is the Moyal star product method [32] based on the Weyl (or Weyl–Wigner) correspondence. From a modern viewpoint the latter method is an example of *deformation theory* [33–35] in which the algebra of functions on the classical phase space is deformed so as to obtain consistency with quantum mechanics. We briefly review the basic principles of deformation theory and explore its relation to the present ICM star product method.

Given the Heisenberg algebra $\mathcal{A}$ of operators $\hat{x}$, $\hat{p}$, and $\hat{e}$ = identity, it is possible to express every sufficiently regular operator $\hat{A}$ in the form [36]

$$\hat{A}(\hat{x}, \hat{p}) = \int_{-\infty}^{\infty} d\sigma \int_{-\infty}^{\infty} d\tau \exp[-i(\sigma\hat{x} + \tau\hat{p})] \alpha(\sigma, \tau), \quad (5.39)$$

where the distribution $\alpha(\sigma, \tau)$ is explicitly obtained from the operator $\hat{A}$ by the trace expression

$$\alpha(\sigma, \tau) = \frac{1}{2\pi} \text{Tr} \{ \hat{A} \exp[i(\sigma\hat{x} + \tau\hat{p})] \}. \quad (5.40)$$

The Fourier transform of $\alpha(\sigma, \tau)$ is defined as

$$A(x, p) = \int_{-\infty}^{\infty} d\sigma \int_{-\infty}^{\infty} d\tau \exp[-i(\sigma x + \tau p)] \alpha(\sigma, \tau). \quad (5.41)$$

The bijection $\hat{A} \mapsto A$ between a suitable class $\{\hat{A}\}$ of operators in $\mathcal{H}$ and a class $\{A\}$ of functions, defined as above, is the *Weyl correspondence* [37, 38]. The functions $A(x, p)$ are formally defined on the dual $\mathcal{A}^*$ of the Heisenberg algebra; in fact this is the classical phase space. Following [34] let us denote this phase space by W .

Under the Weyl correspondence a product of two operators is mapped into the Moyal star product of the mapped functions [32],

$$\hat{A}\hat{B} \mapsto A \star B(x, p), \quad (5.42)$$

where

$$\begin{aligned}
 A * B(x, p) &\equiv \frac{1}{\pi^2} \iiint d\sigma d\sigma' d\tau d\tau' A(x + \sigma, p + \tau) B(x + \sigma', p + \tau') e^{2i(\sigma'\tau - \sigma\tau')} \\
 &= A(x, p) \exp \left[\frac{i}{2} \left(\frac{\tilde{\partial}}{\partial x} \frac{\tilde{\partial}}{\partial p} - \frac{\tilde{\partial}}{\partial p} \frac{\tilde{\partial}}{\partial x} \right) \right] B(x, p) \\
 &= \sum_{m, n=0}^{\infty} \frac{(-1)^n}{m! n!} \left(\frac{i}{2} \right)^{m+n} \frac{\partial^{m+n} A}{\partial x^m \partial p^n} \frac{\partial^{m+n} B}{\partial x^n \partial p^m}.
 \end{aligned} \tag{5.43}$$

It can be shown that the Moyal star product is associative, $A * (B * C) = (A * B) * C$.

The quantum mechanical commutator of two operators is thus mapped into the Moyal bracket

$$[\hat{A}, \hat{B}] \mapsto [A, B]^M \equiv A * B - B * A. \tag{5.44}$$

The Heisenberg equation of motion for an operator is mapped into an equation of similar form for the corresponding mapped function, with the commutator replaced by the Moyal bracket. The functions on the phase space have a similar role in deformation theory as the operators in the Heisenberg picture in quantum mechanics. Indeed, the definition of the star product is equivalent to specifying a particular quantum theory [35].

The general outlines of deformation theory for more complicated symplectic structures and Lie algebras of functions have been discussed, for example, in Refs. [33–35]. Introducing the deformation parameter $\hbar$ (which elsewhere in this paper has been normalized to unity), the ordinary product and the Poisson bracket are deformed to the new structures

$$\begin{aligned}
 f * g &= fg + \mathcal{O}(\hbar), \\
 f * g - g * f &= i\hbar \{f, g\} + \mathcal{O}(\hbar^2).
 \end{aligned} \tag{5.45}$$

The notation implies the usual assumption of the classical limit as $\hbar \rightarrow 0$. A particular class of functions, the preferred functions (or preferred observables), satisfies the latter equation with no second-order anomaly term. All other functions are built from them and can be interpreted to form the universal enveloping algebra of the Lie group generated by the preferred functions. Once a feasible associative star product is constructed, a quantum theory has been created. For example, the Heisenberg algebra necessarily leads to the usual Moyal star product as the only feasible solution of required type. Deformation theory has obvious connections to the theory of quantum groups, which are structures obtained through “quantum” deformations of Lie groups.

The deformed symplectic space has no point-manifold structure, and the formalism leads us into the realm of non-commutative differential geometry [35]. For example, the concepts of states and trajectories do not exist in the same sense as in

the classical case. However, the space of functions on the phase space may still be considered a point-manifold. In this functional phase space (which in Ref. [34] is called N) one may speak of a trajectory which, for example, goes through a particular function f [34].

Although the ICM star product has definite common features with the star product of deformation theory, important differences also occur. First, the ICM star product is defined on a phase space with point-manifold structure. It is not necessary to introduce non-commutative differential geometry, which in deformation theory is conceptually associated with the indeterminacy of quantum mechanics. The ICM dynamics is fully deterministic, just as in classical mechanics (and in full accordance with the deterministic equation of motion of the wave function). Second, the ICM star product is not manifestly associative within the algebra of all (smooth) functions on the ICM phase space. It is associative only in a subalgebra of functions corresponding to observable (measurable) quantities, as defined and discussed above. This derives essentially from the fact that the canonical coordinates in the ICM phase space are themselves not all observables. Third, and this is a very important difference, the ICM star product $A * B$ involves only first-order derivatives of the functions A and B , while the Moyal star product contains derivatives up to infinite order. Indeed, as is obvious from Eqs. (5.43), the Moyal star product involves an integration over the whole phase space W , whereby the ordinary product is multiplied by a factor which is everywhere essentially of the order of unity. In this sense the star product of the deformation theory is very nonlocal in the phase space, whereas the ICM star product is a maximally local deformation of the ordinary product in the ICM phase space. We note further that among the ICM methods only the ECCM is maximally local also in the usual sense of coordinate-space locality. Fourth, while the ICM star product is defined also for functions restricted on the original non-quantized phase space (W), the result $A * B$ (for $A, B \in W$) lies in the full ICM phase space Γ^H . In deformation theory the result would be contained in W . In this sense the ICM is not a subspecies of deformation theory, although the higher-order cluster amplitudes formally are proportional to higher powers of $\hbar$. We remark that the "smallness" of the Planck constant does not mean that the limit $\hbar \rightarrow 0$ in deformation theory is smooth. Indeed, as is stressed in Ref. [34], for example, deformation of the classical Lie algebra is conceptually opposite to the Inönü–Wigner concept of the contraction of a group [39]. The latter typically leads to a drastic change in the topological structure of the group manifold. Similarly, the deformation introduces a change which on the conceptual level does not smoothly vanish as $\hbar \rightarrow 0$. As a matter of fact, even for an arbitrarily small $\hbar$ the physical meaning of the original phase space W remains highly problematic. In the independent cluster formalisms the quantization, which can be formulated using the ICM star product, together with additional concepts concerning the building up of the phase space, performs a mapping of the original phase space W into the ICM phase space Γ^H . If we understand quantization as a relation between "ordinary" manifolds, interesting possibilities may arise with regard to constructing new types of field theories ([21]; see also III).

VI. STRUCTURE OF DIAGRAMS

One of the main advantages of the algebraically formulated ICM methods, and in particular, the intrinsically complicated coupled-cluster approaches, is that they allow vast classes of diagrams to be taken into account in an automatic fashion without a further need to classify them on topological grounds. This is a rather unique feature which does not occur in any other diagrammatical approach, such as Green's function methods, Jastrow-type variational methods, or similar methods. Nevertheless, it is very useful to understand the connection between the algebraic expressions and the diagrams they represent.

Our variational formulation allows the Goldstone diagrams for such quantities as the ground-state energy or ground-state average values of time-independent operators (see, e.g., Ref. [40]) to be grouped as generalized trees, namely the CIM, NCCM or ECCM trees [14, 20, 21]. Each such tree diagram corresponds to a particular infinite set of Goldstone diagrams. In the CIM the branching of the trees is simplest, namely there is only one branch down and one up at every vertex (where we adopt the convention that time evolves in the upward direction); the CIM tree is simply a linear chain. On the other hand, not all of the diagrams in this case are connected. In realistic many-body problems or field theories this leads to difficulties in accounting for the size extensivity of the full sum. In the CIM there are terms which are indeed of arbitrarily high order with respect to the volume or particle number, although these higher-order terms should precisely cancel.

The coupled-cluster methods NCCM and ECCM explicitly sum only connected (or linked; at this level there is no difference in the terminology) diagrams, and thus every term taken separately obeys size extensivity. More precisely, in the NCCM the amplitudes s_n are connected, whereas the amplitudes $\tilde{s}_n$ are not; whereas in the ECCM both the amplitudes σ_n and $\tilde{\sigma}_n$ are connected. The proof of this proposition depends on two parts which we simply sketch here; we are not, however, going to give a full account of the proof, which indeed is more reliably done algebraically, as for example in Appendix A of Ref. [21].

(i) Each vertex of a CCM tree diagram has an internal structure which preserves connectedness once the respective amplitudes (s_n in the case of the NCCM, and σ_n , $\tilde{\sigma}_n$ in the case of the ECCM) joining to the vertex are (internally) connected.

(ii) The top and bottom vertices (i.e., those relatively extremal vertices into which links are joined only from below or from above, respectively) are connected. These vertices appear as inhomogeneous source terms in both the equations of motion and the stationarity conditions for the cluster amplitudes.

These rules guarantee that once the link has originated from a relatively bottom (top or bottom) vertex as connected, it will remain connected when traveling up (arbitrarily up or down) along the NCCM (ECCM) tree diagram.

We shall consider a few illustrative examples. The most general and definitely

sufficient example is the generating functional $A(u, v) = \langle \hat{A}(u, v) \rangle = \langle \exp(ua^\dagger) \exp(va) \rangle$, which itself is the average of an operator ($\hat{A}$) and from which any other operator may be derived. It is given in Eq. (4.8) for the NCCM and in Eq. (4.9) for the ECCM. Let us first consider the NCCM.

We take a particular term of order n in Eq. (4.8) and expand $\tilde{s}$ as a power series of its argument,

$$\tilde{s}(u + x_1 + \cdots + x_n) = \sum_k \tilde{s}_k(u + x_1 + \cdots + x_n)^k.$$

The n th-order term in Eq. (4.8) with the coefficient $\tilde{s}_m$ is thus

$$\begin{aligned} \text{Term}_n^m = & \frac{1}{n!} \tilde{s}_m \int dx_1 \cdots \int dx_n (e^{x_1 v} - 1) \cdots (e^{x_n v} - 1) \\ & \times (u + x_1 + \cdots + x_n)^m \hat{s}(x_1) \cdots \hat{s}(x_n). \end{aligned} \quad (6.1)$$

We may interpret this term as corresponding to a particular NCCM tree diagram, which is the sum of an infinite set of Goldstone diagrams of the general type illustrated by Fig. 1. Each member of this class has (i) a vertex representing the operator ($\hat{A}$), (ii) one box at the top for $\tilde{s}_m$, and (iii) n boxes at the bottom for the clusters s_{ℓ_j} , $j = 1 \cdots n$, where the subscript j refers to the factor $\hat{s}(x_j)$; see Eq. (4.12b). Each factor of u in $\tilde{s}$ corresponds to a line connecting the vertex to $\tilde{s}_m$. Each factor of x_j in $\tilde{s}$ corresponds to a line connecting some cluster s_{ℓ_j} to $\tilde{s}_m$. Each factor of x_j coming from the expansion of $[\exp(x_j v) - 1]$ corresponds to a line connecting the j th cluster s_{ℓ_j} to the vertex; the total number of lines going from all cluster amplitudes $\{s_{\ell_j}\}$ to the vertex thus equals the power of v in a particular term of the expansion. Since each of the factors $[\exp(x_j v) - 1]$ must be at least first order in

FIG. 1. (a) The NCCM tree diagram corresponding to the term of Eq. (6.1). The rectangular box at the top corresponds to the amplitude $\tilde{s}_m$, and the n oval-shaped figures at the bottom to the amplitudes $\{s_{\ell_j}\}$. Time is assumed to proceed upwards. (b) A typical term obtained when the multiconfigurational propagator lines are resolved into multiple single-particle propagator lines. The connectivity is as explained in the main text.

v and thus x_j , there must be at least one line connecting every cluster s_i to the vertex. This is the standard linking requirement of the normal coupled-cluster method [5], and it now arises as a very natural algebraic result. It should perhaps be stressed that for the exponential operator $\hat{A} = \exp(ua^\dagger) \exp(va)$ of Eq. (4.8) the number of up- and down-lines connected to the vertex may be arbitrarily large, because the powers of u and v extend to infinity.

The internal diagrammatic structure of the amplitudes s_n and $\tilde{s}_n$ can be deduced from the equations of stationarity of the energy functional. We do not repeat this analysis here; the result is that only the amplitudes s_n turn out to be fully connected, whereas the amplitudes $\tilde{s}_n$ do not. This behaviour reflects the fact that the amplitudes s_n are additively separable while the amplitudes $\tilde{s}_n$ are multiplicatively separable.

The analysis is fairly similar in the case of the ECCM. We again take the term of n th order from Eq. (4.9),

$$\begin{aligned} \text{Term}_n &= \frac{1}{n!} \int dx_1 \cdots \int dx_n (e^{x_1 v} - 1) \cdots (e^{x_n v} - 1) \\ &\quad \times L_n(u; x_1, \dots, x_n) \hat{\sigma}(x_1) \cdots \hat{\sigma}(x_n), \end{aligned} \quad (6.2)$$

where we have used the notation

$$\begin{aligned} L_n(u; x_1, \dots, x_n) &\equiv \exp[\tilde{\sigma}(u + x_1 + \cdots + x_n) - \tilde{\sigma}(x_1) - \cdots - \tilde{\sigma}(x_n)] \\ &\equiv \exp M_n(u; x_1, \dots, x_n). \end{aligned} \quad (6.3)$$

The special case $L(x, y) \equiv L_2(0; x, y)$ was studied in the previous section. Let us expand the exponent as

$$\begin{aligned} M_n &= \sum_{m=1}^{\infty} \tilde{\sigma}_m M_{nm}(u; x_1, \dots, x_n); \\ M_{nm} &= (u + x_1 + \cdots + x_n)^m - x_1^m - \cdots - x_n^m. \end{aligned} \quad (6.4)$$

Hence

$$\text{Term}_n = \sum_{k_1=0}^{\infty} \sum_{k_2=0}^{\infty} \cdots \text{Term}_n^{k_1 k_2 \cdots}, \quad (6.5)$$

where

$$\begin{aligned} \text{Term}_n^{k_1 k_2 \cdots} &= \frac{1}{n!} \int dx_1 \cdots \int dx_n (e^{x_1 v} - 1) \cdots (e^{x_n v} - 1) \hat{\sigma}(x_1) \cdots \hat{\sigma}(x_n) \\ &\quad \times \prod_{m=1}^{\infty} \frac{1}{k_m!} [\tilde{\sigma}_m M_{nm}(u; x_1, \dots, x_n)]^{k_m}. \end{aligned} \quad (6.6)$$

Referring to Fig. 2, the diagrammatic content of this term can be described as follows. The term again provides an ECCM tree diagram which is a sum of an infinite set of Goldstone diagrams. These are built such that they have (i) k_m boxes at the top for each of the $\tilde{\sigma}_m$ for all m . The diagram naturally also has (ii) the vertex in the middle representing the operator $\hat{A} = \exp(ua^\dagger)\exp(va)$. There are also (iii) n clusters σ_{ℓ_j} at the bottom (towards the past times), from the factors $\hat{\sigma}(x_j)$, see Eq. (4.12a). Each factor of u in L_n corresponds to a link from the vertex to some $\tilde{\sigma}_m$. Each factor of x_j in some M_{nm} corresponds to a line connecting some cluster σ_{ℓ_j} to an $\tilde{\sigma}_m$. Furthermore, just as in the NCCM, each factor of x_j coming from the expansion of $[\exp(x_j v) - 1]$ now corresponds to a line connecting the j th cluster σ_{ℓ_j} to the vertex.

From these rules we can draw several conclusions as to the connectivity structure at a vertex. First, as in the NCCM, each cluster σ_j must be connected to the vertex by at least one line. This is the standard NCCM linking requirement. Second, the form of the multinomials M_{nm} is such that they may contain three types of terms: (i) only powers of u , (ii) powers of u multiplied by powers of x_j , and (iii) only powers of x_j ; these last terms, however cannot have terms that are m th powers of a single variable, such as x_j^m . In case (i) the cluster $\tilde{\sigma}_m$ is connected only to the vertex by m lines. In case (ii) the cluster $\tilde{\sigma}_m$ is connected both to the vertex and to some σ_j 's; it may thus be connected to only one such σ_j . In case (iii) the cluster $\tilde{\sigma}_m$ is not connected to the vertex, but it then must be connected to at least two different cluster amplitudes σ_j . These are the double-linking requirements of the ECCM [14, 21].

If the stationarity conditions (e.g., Eqs. (4.13)) or the equations of motion are used to unravel the diagrammatic content of the ECCM amplitudes $\{\sigma_m, \tilde{\sigma}_m\}$, they all turn out to be connected and thus additively separable, due to the transitivity of the connectivity structure at the vertex.

Finally, let us consider a concrete example. Instead of the exponential operator,

FIG. 2. (a) The ECCM tree diagram corresponding to the term of Eq. (6.6). It has $k + k_2 + \dots$ amplitudes $\tilde{\sigma}_m$ at the top and n amplitudes σ_{ℓ_j} at the bottom, both represented by ovals. (b) A typical term obtained as the multiconfigurational propagator lines are resolved.

FIG 3. The example considered in Eqs. (6.7)–(6.8). This diagram is obtained from the Hamiltonian of the quartic anharmonic oscillator of Eq. (4.11). The four free groups denoted by densely spaced lines have $n_1 = s$, $n_2 = a - s$, $n_3 = c - s - 2$, $n_4 = b + s + 1 - c$ one-particle propagator lines, respectively. The double-linking requirements are such that $n_1 > 0$, $n_2 > 0$, whereas $n_3 \geq 0$, $n_4 \geq 0$.

we focus attention on a polynomial operator, which is obtained by repeated differentiation with respect to u and v , such as the typical term

$$\iint dx_1 dx_2 \exp[\tilde{\sigma}(x_1 + x_2) - \tilde{\sigma}(x_1) - \tilde{\sigma}(x_2)] \times 3k\tilde{\sigma}'(x_1 + x_2) x_1^2 x_2 \tilde{\sigma}(x_1) \tilde{\sigma}(x_2), \quad (6.7)$$

which contributes to the average $k\langle a^\dagger a^3 \rangle$. This is taken from the expectation value (4.11) of the energy of the quartic anharmonic oscillator. Let us consider the terms which are of second order in the amplitudes $\tilde{\sigma}$. These are obtained if the exponential in Eq. (6.7) is expanded out to first order, and using the expansions of Eqs. (6.4), we find

$$\begin{aligned} & 3k \sum_{a=1}^{\infty} \sum_{b=1}^{\infty} b \tilde{\sigma}_a \tilde{\sigma}_b \iint dx_1 dx_2 [(x_1 + x_2)^a - x_1^a - x_2^a] \\ & \quad \times (x_1 + x_2)^{b-1} x_1^2 x_2 \tilde{\sigma}(x_1) \tilde{\sigma}(x_2) \\ & = \sum_{a=1}^{\infty} \sum_{b=1}^{\infty} \sum_{c=1}^{\infty} \sum_{d=1}^{\infty} 3kbc! d! \delta_{c+d, a+b+2} \\ & \quad \times \sum_{s=1}^{a-1} \binom{a}{s} \binom{b-1}{c-s-2} \tilde{\sigma}_a \tilde{\sigma}_b \sigma_c \sigma_d. \end{aligned} \quad (6.8)$$

The corresponding diagrams are drawn in Fig. 3. The interested reader may explicitly verify that the symmetry coefficients of these diagrams are precisely the same as those obtained by more conventional diagrammatic methods.

VII. SUMMARY AND DISCUSSION

We saw already in I that the Bargmann representation provides us with a powerful tool to achieve our aim of giving a complete algebraization of the CIM and CCM parametrizations, at least for the interesting and highly nontrivial class of

models considered, namely single-mode bosonic field theories. In the present paper we have focused attention on the fundamental algebraic structure of the classical phase spaces that arise from each of the CIM, NCCM, and ECCM, and in which the flow is governed by the average-value functional $\bar{H}[x_I, \tilde{x}_I]$ of the relevant cluster amplitudes characterizing each method.

Each of these classical multiconfigurational phase spaces with its classical Hamiltonian is an exact mapping of the original Hilbert space with its quantum-mechanical Hamiltonian operator. Our analysis, for example, has allowed us to give for the first time a purely algebraic description of the abstract topological linking requirements of the CCM parametrizations for the expectation value of the Hamiltonian and other operators. These have hitherto only been described diagrammatically in terms of the pertinent tree diagram structures [14, 20, 21] associated with their (essentially perturbative) expansions. This algebraization process is also of fundamental importance, since it enables us to give a rigorous and exact regularization of the formally badly divergent series that otherwise necessarily appear.

The algebra of observables has been further formalised by introducing an *ICM star product*, which is explicitly studied in the case of the ECCM. The star product is not associative in general. It is associative only in a particular subspace of functions over the phase space, namely the subspace of observables, which therefore is a ring under the combined actions of star multiplication and usual addition. In analogy with the Moyal star product based on the Weyl correspondence, our ICM star product expresses the expectation value of the product of operators in terms of the expectation values of the factor operators and their (functional) derivatives. We point out that while the ICM star product bears a superficial resemblance to the Moyal theory and its generalization, namely *deformation theory*, there also exist important differences which we have carefully described.

We believe that the present investigation of the algebraic structure of the mapped ICM phase spaces is also of special relevance for the ECCM, for reasons explained below. We have seen that only in the ECCM parametrization are *all* of the subsystem cluster amplitudes which fully characterize the quantal many-body or field-theoretic system (namely, $\{\sigma_I, \tilde{\sigma}_I\}$) fully additive, and hence separable, in the sense of obeying the cluster property. Furthermore, this property is preserved at the practical levels of truncation necessary for approximate implementation of the method. This feature is clearly necessary (if not always sufficient) for a realistic description of, for example, topological excitations, where a proper treatment of boundary conditions at infinity is vital. Similar considerations apply to a formulation which is powerful enough, at least in principle, to describe such phenomena as spontaneous symmetry breaking and phase transitions.

To date, formal applications of the ECCM have been made to gauge-field descriptions of both the zero-temperature quantum hydrodynamics of a strongly interacting condensed Bose fluid [41] and a charged impurity in a polarizable medium (of relevance, for example, to the widely used experimental tool of positron annihilation in metals, alloys, and other condensed matter systems) [42]. It is our

hope that the algebraic investigation of the ECCM begun here will not only provide a deeper understanding of the method, but will also widen its sphere of applications to other problems of topical interest in quantum many-body and quantum field theory.

A natural extension of the algebraization programme begun here will be to introduce a set of normal coordinates into the various ICM phase-space manifolds. Thus, such normal-mode coordinates provide the most natural system in terms of which a mathematically well-defined chart can be given for the neighbourhood of the ground state in the abstract CCM phase spaces. The obvious starting-point here is to consider infinitesimal perturbations (e.g., as effected by the linear response to a weak external probe). We have described this procedure in very general terms elsewhere [43] in the specific case of the ECCM, and this investigation will form the starting-point of a subsequent third paper (III) in this series.

Clearly, such normal coordinates can also be introduced in the CC phase spaces for the neighbourhood of an arbitrary state mapped from the original Hilbert space. This is done simply by diagonalizing the second-order part of the Hamiltonian average-value functional expanded around the corresponding point in the classical CC phase space. It is clear that by embarking on such an investigation we will begin to be able to address more global, geometric properties of these manifolds than the more local, algebraic properties discussed here. In particular, we study in III the differential geometry of the NCCM and ECCM phase spaces by considering the connections between the local normal-mode parametrizations for neighbouring points. A particular aim here will be to demonstrate explicitly how the CC phase spaces are genuinely non-Euclidean (i.e., non-flat) as a consequence of the formal, but genuine, underlying nonlinearity of their parametrizations.

Such an outcome is certainly to be expected, not only because of the nonlinearity of the map, but in the present case also because of the intrinsically divergent nature of many of the infinite summations, which therefore drastically affect the structure of the neighbourhood of a point $\{x_i, \tilde{x}_i\}$ through the requirement that the directional derivative of $\bar{H}$ must be regularizable. Also, as we have seen in Sections III and IV, there may exist several distinct image points $p'(s)$, $r = 1, 2, \dots$, in the CCM phase spaces describing the same quantum state $|\Psi(s)\rangle$ in the original Hilbert space, each one corresponding to a different division by the integration line L of the zeros $\{z_m(s)\}$ of the corresponding Bargmann wave function $f(z; s)$. Each such inequivalent choice of a division of the zeros provides a chart of some part of the phase space. The union of all such charts for all CC-representable states in the Hilbert space is an atlas of the entire phase space. The topology of these CCM manifolds is therefore potentially quite complicated. For example, by considering closed circuits in the Hilbert space with respect to some parameter s , beginning and ending, say, with the ground state $|\Psi_0\rangle$, it turns out that the CCM phase spaces can display, for example, the phenomenon of *geometric phase* or *(an)holonomy* [44]. A more detailed discussion of these and other geometrical and topological aspects of the structure of the classical CCM phase spaces is deferred to the subsequent paper (III).

APPENDIX A: ASYMPTOTIC PROPERTIES OF CERTAIN FUNCTIONS

In this appendix we intend to study the asymptotic properties of the ratio functions

$$r_n(ix) = \frac{f^n(ix)}{f^0(ix)}, \quad (\text{A.1})$$

$$\tilde{r}_{mn}(x) = \frac{\tilde{s}^{mn}(x)}{\tilde{s}^{00}(x)}, \quad (\text{A.2})$$

for large $|x| \rightarrow \infty$ in the region $\arg x \approx 0$, where these functions are needed. In particular we wish to establish the influence of the energy eigenvalues E_n on the asymptotic properties.

To this end we first examine the asymptotic properties of the Schrödinger eigenfunctions $\psi_n(x)$. If we write them in the usual WKB representation,

$$\psi_n(x) = e^{Q_n(x)}, \quad (\text{A.3})$$

we easily derive from the Schrödinger equation (3.11) the relation,

$$Q_n''(x) + Q_n'(x)^2 = x^2 + 2kx^{2K} - 2E_n. \quad (\text{A.4})$$

It is now straightforward to show that Q_n' has the expansion,

$$Q_n'(x) \xrightarrow{x \rightarrow \infty} a_0 x^K + a_1 x^{2-K} + a_2 x^{-K} + \dots + b_0 x^{-1} + \dots, \quad (\text{A.5})$$

where $a_0 = -\sqrt{2k}$ and that the leading energy-dependent coefficient is a_2 in all cases. The result can be put in the form (to within a constant for the overall normalization factor)

$$Q_n(x) \xrightarrow{x \rightarrow \infty} Q_0(x) - \frac{E_n}{(K-1)} (2k)^{-1/2} x^{1-K}, \quad (\text{A.6})$$

where $Q_0(x)$ is independent of the index n and its leading asymptotic behaviour is given by

$$Q_0(x) \xrightarrow{x \rightarrow \infty} -\frac{\sqrt{2k}}{(K+1)} x^{K+1} - \frac{\delta_{K,2}}{2\sqrt{2k}} x - \frac{1}{2} K \ln x + \dots \quad (\text{A.7})$$

In order to examine the asymptotic properties for real values of x of the function $r_n(ix)$ given by Eq. (A.1), we use the integral representation of $\phi^n(ix)$ from Eq. (3.13),

$$\phi^n(ix) = \pi^{-1/4} \int_{-\infty}^{\infty} dy \exp[\sqrt{2} ixy - \frac{1}{2} y^2 + Q_n(y)]. \quad (\text{A.8})$$

In the limit $x \rightarrow \infty$, it is easily verified from Eqs. (A.4) and (A.5) that the exponent in the integral in Eq. (A.8) may be stationary at the points y_c , where

$$y_c^K \xrightarrow{x \rightarrow \infty} \pm ix/\sqrt{k}, \quad (\text{A.9})$$

and the plus sign must be chosen at least within the sector $|\arg y| < 3\pi/2(K+1)$ surrounding the real y -axis. It is a simple matter to show that out of the possible roots to Eq. (A.9), the dominant one for the usual saddle-point analysis of Eq. (A.8) takes the particular value,

$$y_c \xrightarrow{x \rightarrow \infty} k^{-1/2K} \exp\left(\frac{i\pi}{2K}\right) x^{1/K}. \quad (\text{A.10})$$

Straightforward analysis then shows that the asymptotic behaviour of $\phi^n(ix)$ is given by

$$\phi^n(ix) \xrightarrow{x \rightarrow \infty} \text{const} \times \exp \left\{ T_0(x) - \frac{\varepsilon_n}{(K-1)} 2^{-1/2} k^{-1/2K} e^{i(\pi/2)((1-K)/K)} x^{(1-K)/K} \right\}, \quad (\text{A.11})$$

where $T_0(x)$ is independent of the index n and has leading asymptotic behaviour, in agreement with Eqs. (3.16) and (3.17), given by

$$T_0(x) \xrightarrow{x \rightarrow \infty} -\frac{\sqrt{2}K}{(K+1)} k^{-1/2K} e^{i(\pi/2)((1-K)/K)} x^{(K+1)/K}. \quad (\text{A.12})$$

Hence, we readily find for real values of $x \rightarrow \infty$ the final result,

$$\left| \frac{f^n(ix)}{f^0(ix)} \right| = \left| \frac{\phi^n(ix)}{\phi^0(ix)} \right| = |r_n(ix)| \xrightarrow{x \rightarrow \infty} \text{const} \times \exp \left\{ -\frac{\varepsilon_n}{N(K)} x^{(1-K)/K} \right\}, \quad (\text{A.13})$$

where

$$N(K) \equiv \sqrt{2}(K-1) k^{1/2K} \text{cosec}(\pi/2K). \quad (\text{A.14})$$

It is, hence, clear from Eq. (A.13) that the function $r_n(ix)$ approaches a constant value as $x \rightarrow \infty$, since $K > 1$.

We now turn our attention to the function $\tilde{s}^{mn}(x)$ in order to examine similarly the asymptotic properties for real values of x of the ratio function $\tilde{r}_{mn}(x)$. By denoting $u = z/(2\sqrt{2})$, we may rewrite the integral representation of Eq. (3.40) in the form

$$\tilde{s}^{mn}(z) = \text{const} \times \int dx \exp \{ Q_m(u+x) + Q_n(u-x) + 2ux \}, \quad (\text{A.15})$$

since the wave function $\tilde{\psi}_m(x)$ is real. In the limit $u \rightarrow \infty$ the integrand has a strongly peaked maximum around

$$x_c \approx (K \sqrt{2k})^{-1} u^{2-\kappa}, \quad (\text{A.16})$$

which can be sufficiently accurately approximated by $x_c \approx 0$. By the saddle-point method we therefore can estimate the result of the integration, and by including terms up to the level of the first energy-dependent contributions we obtain

$$\tilde{s}^{mn}(z) = \text{const} \times \exp \left\{ 2Q_0(u) - \frac{(\varepsilon_m + \varepsilon_n)}{(K-1)\sqrt{2k}} u^{1-\kappa} \right\}. \quad (\text{A.17})$$

Finally, by resubstituting the variable z , we obtain

$$\tilde{r}_{mn}(z) = \frac{\tilde{s}^{mn}(z)}{\tilde{s}^{00}(z)} \xrightarrow{z \rightarrow x} \text{const} \times \exp \left\{ -\frac{(\varepsilon_m + \varepsilon_n)}{(K-1)\sqrt{2k}} 2^{(3/2)(K-1)} z^{1-\kappa} \right\}. \quad (\text{A.18})$$

This clearly approaches a constant, because the power of z in the exponent is negative, and in the non-leading terms it is even more negative.

These results also prove the existence and convergence of the integrals needed in calculating the expansions and matrix elements to be discussed in paper III.

APPENDIX B: NON-UNIQUENESS OF THE AMPLITUDES $\{\sigma_n\}$

As explained in the main text, each inequivalent line L used to define $\hat{s}(x)$ corresponds to a different chart of the neighbourhood of the point in the CCM manifold. To substantiate this claim we rewrite the second of Eqs. (3.53a) as

$$x\hat{s}(x) = \int_L \frac{d\zeta}{2\pi i} e^{-x\zeta s'(\zeta)} \quad (x \in L'). \quad (\text{B.1})$$

As discussed in I, using the Weierstrass-Hadamard decomposition of the holomorphic wave function $f(z)$, we can write

$$s'(z) = -z + f_1 + \sum_m \left(\frac{1}{z - z_m} + \frac{1}{z_m} \right), \quad (\text{B.2})$$

where $\{z_m\}$ are the zeros of $f(z)$. The integration in Eq. (B.1) is straightforward to perform with the explicit result,

$$\begin{aligned} x\hat{s}(x) = & \delta'_{L'}(x) + f_1 \delta_{L'}(x) + \sum_m^+ \left[\theta_{L'}(-x) e^{-xz_m} + \frac{1}{z_m} \delta_{L'}(x) \right] \\ & + \sum_m^- \left[-\theta_{L'}(x) e^{-xz_m} + \frac{1}{z_m} \delta_{L'}(x) \right] \quad (x \in L'). \end{aligned} \quad (\text{B.3})$$

As in I, the sum over zeros is divided into two terms corresponding to those zeros that are to the left (+) or to the right (−) of the line $L = a + \eta \mathbf{R}$. We recall that since the argument $x \in L'$, it is of form $x = \pm \eta' |x|$. For a complex argument the step function and the Dirac delta have to be interpreted such that $\theta_L(\eta' y) = \theta(y) \equiv \frac{1}{2}(1 + \text{sgn } y)$, $\delta_L(\eta' y) = (\eta')^{-1} \delta(y)$. If we denote $x = \eta' y$, where y is real, it is easily shown that asymptotically $\hat{s}(x)$ has the properties

$$\begin{aligned} |x \hat{s}(x) e^{xa}| &\xrightarrow{y \rightarrow -\infty} \text{const} \times \exp(d^+ y); \\ |x \hat{s}(x) e^{xa}| &\xrightarrow{y \rightarrow \infty} \text{const} \times \exp(-d^- y), \end{aligned} \quad (\text{B.4})$$

where d^+ and d^- are the distances from the line L of the nearest zero of $f(z)$ on the left-hand and the right-hand sides of L , respectively.

Written in this way the function $x \hat{s}(x) e^{xa}$ is a regularized generalized function [29] and is thus maximally analytic around the special point $x=0$. The non-analyticity at $x=0$ can be thought of as being represented by two nonanalytic regions, such as cuts or poles, that are shifted aside from the special point but extend very close to it. The function $x \hat{s}(x)$ can therefore be considered as an analytic function (in the limiting sense) in a finite strip in the complex x plane, including the origin. For example, if the angle ϕ of the line L can vary in the range $\phi_1 < \phi < \phi_2$ without crossing any zeros, the function $x \hat{s}(x)$ is analytic in the pair of opposite sectors $\pi/2 - \phi_2 < \arg x < \pi/2 - \phi_1$ and $3\pi/2 - \phi_2 < \arg x < 3\pi/2 - \phi_1$ and in the neighbourhood of $x=0$ connecting these sectors. On the other hand, for an inequivalent line L that divides the zeros differently, $x \hat{s}(x)$ will be defined in a different pair of opposite sectors as a function that is not an analytic continuation of its previous definition in the other pair of sectors.

Keeping this in mind, it is obvious that all integrals involving the functions $\hat{s}(x)$ or $\hat{\sigma}(x) = \hat{s}(x) \tilde{s}(x)$ that appear in the main text can be interpreted as integrals over functions that are analytic on, and in a finite neighbourhood of, the integration line L' , which means that the slope of the route L' can be slightly varied, in accordance with the corresponding variations of the line L in the complex z plane. Thus, e.g., the function $\sigma(z)$ of Eq. (3.55), as well as the expansion coefficients $\{\sigma_n\}$ of Eq. (4.12a), must be independent of the slope of L and sensitive only to the differing ways to divide the zeros by the line. This particular case is actually very clearly seen from the equivalent definition in Eq. (3.56).

APPENDIX C: EXAMPLE: THE SQUEEZED HARMONIC OSCILLATOR

In order to illustrate the Bargmann-space formalism for the two CCM representations, we consider the exactly soluble example of the “squeezed” harmonic oscillator with Hamiltonian,

$$\begin{aligned} H &= H(\hat{x}, \hat{p}) = \frac{1}{2} (1 - 2\lambda) \hat{p}^2 + \frac{1}{2} (1 + 2\lambda) \hat{x}^2 \\ &= H(a^\dagger, a) = \frac{1}{2} + a^\dagger a + \lambda(a^{\dagger 2} + a^2), \quad 0 < \lambda < \frac{1}{2}. \end{aligned} \quad (\text{C.1})$$

In the case of antisqueezing, $\lambda < 0$, which we do not handle, the integration routes in the subsequent equations would have to be chosen differently, but otherwise the treatment would be quite analogous. Equation (4.3) immediately yields the NCCM energy expectation value,

$$\begin{aligned}\bar{H}^{\text{NCCM}} &= \int_{-\infty}^{\infty} \frac{dx}{2\pi} \tilde{s}_F(x) H\left(ix, -i \frac{d}{dx} + \varrho(x)\right) \\ &= \int_{-\infty}^{\infty} \frac{dx}{2\pi} \tilde{s}_F(x) \left[\frac{1}{2} + ix\varrho(x) - \lambda x^2 - i\lambda\varrho'(x) + \lambda\varrho^2(x) \right],\end{aligned}\quad (\text{C.2})$$

where

$$\varrho(x) = s'(ix). \quad (\text{C.3})$$

The stationary NCCM amplitude functions $\{s^n(z), \tilde{s}^n(z)\}$ are now obtained by requiring that $\bar{H}^{\text{NCCM}}$ be stationary with respect to arbitrary variations in $\{s(x), \tilde{s}(x)\}$, or equivalently $\{\varrho(x), \tilde{s}_F(x)\}$, subject to the constraint

$$\tilde{s}(0) = \int_{-\infty}^{\infty} \frac{dx}{2\pi} \tilde{s}_F(x) = 1. \quad (\text{C.4})$$

We thus have the two constrained variational equations,

$$ix\tilde{s}_F^n(x) + i\lambda\tilde{s}_F^{n'}(x) + 2\lambda\varrho_n(x)\tilde{s}_F^n(x) = 0, \quad (\text{C.5})$$

$$\frac{1}{2} + ix\varrho_n(x) - \lambda x^2 - i\lambda\varrho_n'(x) + \lambda\varrho_n^2(x) = E_n, \quad (\text{C.6})$$

where

$$\varrho_n(x) = s^{n'}(ix). \quad (\text{C.7})$$

The Lagrange multiplier E_n in Eq. (C.6), which arises from the constraint (C.4), is readily seen from Eqs. (C.2) and (C.4) to be simply the stationary energy eigenvalue of the n th state.

By making the simple substitution,

$$\varrho_n(x) \equiv -i \frac{u_n'(x)}{u_n(x)}, \quad (\text{C.8})$$

the nonlinear first-order Riccati equation (C.6) is transformed into the second-order linear equation

$$-\lambda u_n''(x) + xu_n'(x) - \lambda x^2 u_n(x) = (E_n - \frac{1}{2}) u_n(x). \quad (\text{C.9})$$

Furthermore, it is trivial to solve Eqs. (C.5) and (C.4) for $\tilde{s}_F^n(x)$ in terms of $u_n(x)$ as

$$\tilde{s}_F^n(x) = C_n^{-1} u_n^2(x) e^{-(1/2)x^2/\lambda}, \quad C_n \equiv \int_{-\infty}^{\infty} \frac{dx}{2\pi} u_n^2(x) e^{-(1/2)x^2/\lambda}. \quad (\text{C.10})$$

It is now convenient to make the further substitution

$$u_n(x) \equiv e^{(1/2)\kappa x^2} p_n(x), \quad (\text{C.11})$$

where κ is at present arbitrary. Substitution of Eq. (C.11) into Eq. (C.9) yields the differential equation

$$-\lambda p_n''(x) + (1 - 2\kappa\lambda) x p_n'(x) - (\lambda - \kappa + \lambda\kappa^2) x^2 p_n(x) = (E_n - \frac{1}{2} + \kappa\lambda) p_n(x). \quad (\text{C.12})$$

If we now make the specific choice

$$\kappa \equiv \frac{1 - \sqrt{1 - 4\lambda^2}}{2\lambda}, \quad (\text{C.13})$$

whence $0 \leq \kappa < 1$, Eq. (C.12) reduces to the simpler equation,

$$-\lambda p_n''(x) + \omega x p_n'(x) = (E_n - \frac{1}{2}\omega) p_n(x) \quad (\text{C.14})$$

$$\omega \equiv \sqrt{1 - 4\lambda^2}, \quad (\text{C.15})$$

in terms of the solution to which we have from Eqs. (C.8), (C.10), and (C.11),

$$s^n(z) = -\frac{1}{2} \kappa z^2 + \ln p_n(-iz) + \text{const}, \quad (\text{C.16})$$

$$\tilde{s}_F^n(z) = C_n^{-1} p_n^2(z) \exp\left(-\frac{\omega z^2}{2\lambda}\right), \quad C_n = \int_{-\infty}^{\infty} \frac{dx}{2\pi} p_n^2(x) \exp\left(-\frac{\omega x^2}{2\lambda}\right). \quad (\text{C.17})$$

It is easy to verify from Eq. (C.14) that the leading asymptotic behaviour of $p_n(x)$ for large values of $|x|$ is $p_n(x) \propto \exp(bx^2)$, where $b=0$ and $b=\omega/(2\lambda)$ for the two independent solutions. It is clear that the latter solution with $b=\omega/(2\lambda)$ is forbidden since the integral in Eq. (C.17) then diverges. Hence, $p_n(x)$ is an n th-order polynomial in x , and it is trivial to verify from Eq. (C.14) that the eigenvalue E_n is then given by

$$E_n = (n + \frac{1}{2}) \omega. \quad (\text{C.18})$$

Furthermore, the corresponding eigenfunction $p_n(x)$ is readily shown to be expressible in the form

$$p_n(x) = \text{const} \times \left(x - \frac{\lambda}{\omega} \frac{d}{dx}\right)^n 1. \quad (\text{C.19})$$

Either from this equation or from the differential equation (C.14) we may deduce that, by definition, the polynomials p_n are Hermite polynomials [45],

$$p_n(z) = \text{const} \times H_n(\tau z), \quad \tau = \sqrt{\omega/2\lambda}. \quad (\text{C.20})$$

Equation (C.16) shows that the CIM Bargmann eigenfunction is given by

$$\begin{aligned} f^n(z) &= \text{const} \times H_n(-itz) e^{-\kappa z^2/2} \\ &= \text{const} \times e^{-\kappa z^2/2} \left(z + \frac{\lambda}{\omega} \frac{d}{dz} \right)^n 1. \end{aligned} \quad (\text{C.21})$$

By making use of the trivial operator relation

$$e^{-\kappa z^2/2} \frac{d}{dz} e^{\kappa z^2/2} = \frac{d}{dz} + \alpha z, \quad (\text{C.22})$$

one may show that Eq. (C.21) may also be written in the alternative form,

$$f^n(z) = \text{const} \times \left(z + \kappa \frac{d}{dz} \right)^n e^{-\kappa z^2/2}. \quad (\text{C.23})$$

We may also calculate the Fourier transform of $f^n(z)$ from Eq. (C.23) as

$$f_F^n(z) = \text{const} \times \int_{-\infty}^{\infty} dx e^{-ixz} \left(x + \kappa \frac{d}{dx} \right)^n e^{-\kappa x^2/2}. \quad (\text{C.24})$$

By repeated integration by parts and recalling that $\kappa > 0$ from its definition in Eq. (C.13), we obtain

$$\begin{aligned} f_F^n(z) &= \text{const} \times \int_{-\infty}^{\infty} dx e^{-\kappa x^2/2} \left(x - \kappa \frac{d}{dx} \right)^n e^{-ixz} \\ &= \text{const} \times \left(i \frac{d}{dz} + i\kappa z \right)^n \int_{-\infty}^{\infty} dx e^{-(1/2)\kappa x^2 - ixz} \\ &= \text{const} \times \left(i \frac{d}{dz} + i\kappa z \right)^n e^{-z^2/2\kappa}. \end{aligned} \quad (\text{C.25})$$

A further use of Eq. (C.22) gives the final result,

$$\begin{aligned} f_F^n(z) &= \text{const} \times e^{-z^2/2\kappa} \left(i \frac{d}{dz} - i \frac{\omega}{\lambda} z \right)^n 1 \\ &= \text{const} \times H_n(\tau z) e^{-\tau^2 z^2/2}. \end{aligned} \quad (\text{C.26})$$

Equations (C.17), (C.21), and (C.26) verify that

$$\begin{aligned} \tilde{s}_F^n(z) &= \tilde{f}_F^n(z) f^n(iz) \\ &= 2\pi\tau (\sqrt{\pi} 2^n n!)^{-1} H_n(\tau z)^2 e^{-\tau^2 z^2}, \end{aligned} \quad (\text{C.27})$$

as required, by comparison with Eq. (C.17). Using the well-known properties of

Hermite polynomials the normalization coefficient in the above formula is easily verified.

The inverse Fourier transform of $\tilde{s}_F^n(z)$ can also be found in closed form. From Eqs. (3.21) and (C.27) we have

$$\tilde{s}^n(z) = (\sqrt{\pi} 2^n n!)^{-1} \int_{-\infty}^{\infty} dy e^{iyz/\tau} H_n(y)^2 e^{-y^2}. \quad (C.28)$$

By making use of the generating function for the Hermite polynomials [45],

$$e^{-s^2 + 2sx} = \sum_{n=0}^{\infty} \frac{1}{n!} s^n H_n(x), \quad (C.29)$$

we readily derive the relation

$$\tilde{s}^n(\tau z) = (\sqrt{\pi} 2^n n!)^{-1} \partial_u^n \partial_v^n \int_{-\infty}^{\infty} dy e^{iyz - y^2} e^{-u^2 - v^2 + 2(u+v)y} \Big|_{u=v=0}.$$

The remaining integral is trivially evaluated to yield the relation

$$\tilde{s}^n(\tau z) = (2^n n!)^{-1} e^{-(1/4)z^2} \partial_u^n \partial_v^n e^{2uv + iz(u+v)} \Big|_{u=v=0},$$

from which it follows that

$$\begin{aligned} \tilde{s}^n(\tau z) &= (2^n n!)^{-1} e^{-(1/4)z^2} \partial_u^n (2u + iz)^n e^{(2v+iz)u} \Big|_{u=v=0} \\ &= e^{-(1/4)z^2} \sum_{m=0}^n \binom{n}{n-m} \frac{1}{m!} \left(-\frac{1}{2}z^2\right)^m. \end{aligned} \quad (C.30)$$

Equation (C.30) is most simply given in terms of Laguerre polynomials [45] to yield

$$\tilde{s}^n(z) = \exp\left(-\frac{z^2}{4\tau^2}\right) L_n\left(\frac{z^2}{2\tau^2}\right). \quad (C.31)$$

The ECCM amplitude $\tilde{\sigma}^n = \ln \tilde{s}^n$ is therefore trivially given as

$$\tilde{\sigma}^n(z) = -\frac{z^2}{4\tau^2} + \ln L_n\left(\frac{z^2}{2\tau^2}\right). \quad (C.32)$$

This function is analytic everywhere except for logarithmic branch cut singularities on the real z -axis. None of them, however, is precisely at the origin.

We note that the polynomials $H_n(z)$ are even (odd) functions of z when n is even (odd). Hence, for the even eigenfunctions $n=2m$ we can normalize $s^n(z)$ so that $s^n(0)=0$ by writing

$$s^n(z) = -\frac{1}{2} \kappa z^2 + \ln \left(\frac{H_n(-itz)}{H_n(0)} \right), \quad n = 0, 2, \dots \quad (C.33)$$

The odd eigenfunctions have a zero at the origin, $H_{2m+1}(0)=0$, and we must abandon the requirement that $s(0)=0$; we must, for example, ignore the denominator under the logarithm function in the above formula. As discussed in Sections III–IV, this has no consequences for the CC methods, because only the derivative function $s'(z)$ is relevant.

Finally, we may also calculate the corresponding ECCM functions $\{\sigma''(z), \tilde{\sigma}''(z)\}$ for the present example. Applying Eqs. (4.6) and (4.9) we easily derive the energy,

$$\begin{aligned} \bar{H} = & \frac{1}{2} + \int dx \tilde{\sigma}'(x) x \hat{\sigma}(x) + \lambda \int dx \delta(x) [\tilde{\sigma}''(x) + \tilde{\sigma}'(x)^2] + \lambda \int dx x^2 \hat{\sigma}(x) \\ & + \lambda \iint dx_1 dx_2 e^{\tilde{\sigma}(x_1+x_2) - \tilde{\sigma}(x_1) - \tilde{\sigma}(x_2)} x_1 x_2 \hat{\sigma}(x_1) \hat{\sigma}(x_2). \end{aligned} \quad (\text{C.34})$$

The requirement of stationarity against small variations of the canonical amplitudes $\hat{\sigma}(x)$ and $\tilde{\sigma}(x)$ gives the following conditions:

$$\frac{\delta \bar{H}}{\delta x \hat{\sigma}(x)} = \tilde{\sigma}'(x) + \lambda x + 2\lambda \int dy e^{\tilde{\sigma}(x+y) - \tilde{\sigma}(x) - \tilde{\sigma}(y)} y \hat{\sigma}(y) = 0; \quad (\text{C.35})$$

$$\begin{aligned} \frac{\delta \bar{H}}{\delta \tilde{\sigma}(x)} = & -\frac{d}{dx} [x \hat{\sigma}(x)] + \lambda \tilde{\sigma}''(x) - 2\lambda \frac{d}{dx} [\delta(x) \tilde{\sigma}'(x)] \\ & + \lambda \int dy e^{\tilde{\sigma}(x) - \tilde{\sigma}(x-y) - \tilde{\sigma}(y)} (x-y) y \hat{\sigma}(x-y) \hat{\sigma}(y) \\ & - 2\lambda \int dy e^{\tilde{\sigma}(x+y) - \tilde{\sigma}(x) - \tilde{\sigma}(y)} xy \hat{\sigma}(x) \hat{\sigma}(y) \\ = & A \delta(x). \end{aligned} \quad (\text{C.36})$$

The delta-function term with an unspecified coefficient on the last row of the latter equation results from the boundary condition $\tilde{\sigma}(0)=0$, which is a consequence of the normalization requirement $\tilde{s}(0)=1$.

The most straightforward method—and in the present case, indeed, perhaps the only one—to solve the above equations is to transform them into linear equations. This is possible in the present case, just as it was possible in the NCCM case considered above. Not unexpectedly, we therefore introduce the functions $\tilde{s}(x) = \exp \tilde{\sigma}(x)$ and $\hat{s}(x) = \hat{\sigma}(x)/\tilde{s}(x)$, in terms of which the equations can be considerably simplified. By multiplying Eq. (C.35) with $\tilde{s}(x)$ we find, after simplification,

$$\tilde{s}'(x) + \lambda x \tilde{s}(x) + 2\lambda \int dy \tilde{s}(x+y) y \hat{s}(y) = 0. \quad (\text{C.37})$$

The Fourier transform of this equation is precisely the first of the NCCM equations, Eq. (C.5), if the transform of $x \hat{s}(x)$ is identified with the function $\varrho(x)$.

On the other hand, by forming a suitable combination of Eqs. (C.35) and (C.36) and simplifying, we find

$$\begin{aligned} \frac{\delta \bar{H}}{\delta \bar{\sigma}(x)} + x \bar{\sigma}(x) \frac{\delta \bar{H}}{\delta x \bar{\sigma}(x)} &= -\tilde{s}(x) \frac{d}{dx} [x \hat{s}(x)] + \lambda \delta''(x) - 2\lambda \tilde{s}'(0) \delta'(x) \\ &\quad + \lambda \tilde{s}(x) x^2 \hat{s}(x) + \lambda \tilde{s}(x) \int dy (x-y) y \hat{s}(x-y) \hat{s}(y) \\ &= A \delta(x). \end{aligned} \quad (\text{C.38})$$

Using the following well-known properties of the delta-function,

$$\begin{aligned} \delta(x) f(x) &= \delta(x) f(0), \\ \delta'(x) f(x) &= \delta'(x) f(0) - \delta(x) f'(0), \\ \delta''(x) f(x) &= \delta''(x) f(0) - 2\delta'(x) f'(0) + \delta(x) f''(0), \end{aligned} \quad (\text{C.39})$$

we may divide Eq. (C.38) by $\tilde{s}(x)$ and obtain

$$-\frac{d}{dx} [x \hat{s}(x)] + \lambda \delta''(x) + \lambda x^2 \hat{s}(x) + \lambda \int dy (x-y) y \hat{s}(x-y) \hat{s}(y) = A' \delta(x), \quad (\text{C.40})$$

where $A' = A + \lambda \tilde{s}''(0)$. The last term on the left-hand side is a convolution, for which reason it is advantageous to form the Fourier transform of the equation. In this way, denoting again the transform of $x \hat{s}(x)$ by $\varrho(x)$, we derive the second of the NCCM equations, Eq. (C.6).

In Eq. (C.32) we already found the ECCM amplitude $\bar{\sigma}''(z)$. The other canonical amplitude $\sigma(z)$ or $\hat{\sigma}(x)$ cannot readily be obtained in closed form. We apply Eq. (3.56b) in the following form and take results from Eqs. (C.27) and (C.33):

$$\begin{aligned} \sigma''(z) &= \int_L \frac{du}{2\pi i} \tilde{s}_F^n(iz - iu) s''(u) \\ &= 2\pi\tau (\sqrt{\pi} 2^n n!)^{-1} \int_L \frac{du}{2\pi i} \exp[\tau^2(z-u)^2] \\ &\quad \times H_n(i\tau(z-u))^2 \left[-\kappa u - i\tau \frac{H'_n(-i\tau u)}{H_n(-i\tau u)} \right]. \end{aligned} \quad (\text{C.41})$$

This is easily computed for the ground state, in which case we obtain the result

$$\sigma^0(z) = -\frac{1}{2} \kappa z^2. \quad (\text{C.42})$$

For the excited states there is no obvious simplification.

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