Independent-Cluster Parametrizations of Wave Functions in Model Field Theories. I. Introduction to Their Holomorphic Representations

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The configuration-interaction method (CIM), normal coupled-cluster method (NCCM), and extended coupled-cluster method (ECCM) form a rather natural hierarchy of formulations of increasing sophistication for describing interacting systems of quantum-mechanical particles or fields. They are denoted generically as independent-cluster (IC) parametrizations in view of the way in which they incorporate the many-body correlations via sets of amplitudes that describe the various correlated clusters within the interacting system as mutually independent entities. They differ primarily by the way in which they incorporate the exact locality and separability properties. Each method is shown to provide, in principle, an exact mapping of the original quantum-mechanical problem into a corresponding classical Hamiltonian mechanics in terms of a set of multiconfigurational canonical field amplitudes. In perturbation-theoretic terms the IC methods incorporate infinite classes of diagrams at each order of approximation. The diagrams differ in their connectivity or linkedness properties. The structure of the ECCM in particular makes it capable of describing such phenomena as phase transitions, spontaneous symmetry breaking, and topological states. We address such fundamentally important questions as the existence and convergence properties of the three IC parametrizations by formulating the holomorphic representation of each one for the class of single-mode bosonic field theories which include the anharmonic oscillators. These highly nontrivial models provide a stringent test for the coupled-cluster methods. We present a particularly detailed analysis of the asymptotic behaviour of the various amplitudes which exactly characterize each IC method. More generally, the holomorphic representation allows us to give a completely algebraic description of all aspects of each scheme. In particular, this includes the topological connectivity properties of the various terms or diagrams in their expansions. We construct a generating functional for the calculation of the expectation values of arbitrary operators for each of the IC parametrizations. The functional is used in each case to formulate the quantum mechanical action principle and to perform the mapping into the corresponding classical phase space. © 1991 Academic Press, Inc.

I. INTRODUCTION

In order to describe quantum many-body systems and their properties, various methods have been developed which aim to go beyond perturbation theory. Nevertheless, there are relatively few basically different techniques that are fundamental in the sense of being both applicable to a wide variety of physical systems and capable in principle of systematic improvement, and which at the same time yield in practice results of high precision at reasonably low levels of truncation [1]. Two typical such classes of techniques are: (i) variational techniques based on wave functions of the Jastrow or Jastrow-Feenberg form, and their systematic improvement via the method of correlated basis functions [2-5]; and (ii) the configuration-interaction method [6], which in its simplest form diagonalizes the Hamiltonian in a finite subspace of the full many-body Hilbert space, and its necessary adaption for extended systems via coupled cluster (CC) techniques [7-15].

It is this latter class of techniques with which we are concerned in the present paper. We refer to them collectively as independent-cluster (IC) methods. More specifically, they include the three methods: (i) the configuration-interaction method (CIM) [6]; (ii) the normal coupled-cluster method (NCCM) [1, 7-12, 14, 15]; and (iii) the extended coupled-cluster method (ECCM) [13, 16, 17]. Each starts from its own distinct parametrization of the many-body wave function. What characterizes the IC methods generically is the way that the many-body correlations are incorporated into these parametrizations in terms of sets of amplitudes which describe the various correlated clusters or configurations of subsystems within the full interacting system.

Thus, the operators that generate these subsystems, and whose matrix elements give the corresponding amplitudes, form a bicommuting set of operators. More specifically, the algebra of all operators in the full many-body Hilbert space $\mathcal{H}$ is decomposed into two Abelian subalgebras of creation and destruction operators, respectively. These are defined with respect to some suitably chosen model state or reference state which thus plays the role of a cyclic vector. A cyclic ket vector, for example, is one from which all other ket vectors in the Hilbert space $\mathcal{H}$ can be generated by operating on it with elements of the algebra of creation operators. The mutual commutativity of the creation operators for the associated ket-state configurations, and similarly for the destruction operators for the associated bra-state configurations, then leads directly to the concept of the *mutual independence* of the various clusters within each of the two subsets, and hence to our chosen nomenclature of *independent-cluster* techniques. By contrast, the well-known Jastrow trial form of the wavefunction which includes pairwise correlations only, can also be written in terms of an (exponential) operator acting on a model state, but in this case the various terms in the exponent do *not* commute with each other.

One of the most interesting features of the IC techniques is that they each provide an exact mapping of the original quantum many-body theory in $\mathcal{H}$ into a classical Hamiltonian mechanics in some well-defined complex symplectic phase space for the particular set of many-body, classical (c-number), configuration-space

amplitudes that characterize a given method, and which play the role of generalized mean fields. In each case this mapping arises ultimately from a one-to-one correspondence between commutators in the original Hilbert space $\mathcal{H}$ and suitably defined generalized Poisson brackets in the corresponding classical phase space. Where the three IC methods principally differ from each other is in their connectedness or linkedness properties for these characteristic complete sets of amplitudes. In turn, these properties are intimately related to the separability feature of the exact many-body wave function in the dissociation limit where the system is split into two asymptotically free fragments, and whether and at what level this feature is incorporated into each particular IC parametrization.

Thus, for example, whereas the CIM contains disconnected diagrams for the ground-state energy expectation value, and thereby suffers from the so-called size-extensivity or size-consistency problems [18], both CC methods specifically incorporate the Goldstone linked-cluster theorem [19]. Furthermore, none of the individual amplitudes in the CIM is a linked-cluster quantity in the sense of obeying the cluster property, namely that it becomes asymptotically zero in the limit that any one particle or group of particles from those described by the particular configuration amplitude becomes far removed in real space from the remainder. In the NCCM by comparison, each member of one of the two subsets of amplitudes obeys the cluster property, whereas those of the other subset do not. Only in the ECCM is the important cluster property obeyed by *all* of the characteristic amplitudes.

These connectivity properties of the various amplitudes manifest themselves in definite locality (or, more precisely, quasilocality) properties for the corresponding mapped classical Hamiltonian theory. Whereas the classical phase space for each of the three IC methods is equally complicated a priori, the increasing degree of incorporation of the full locality and separability aspects along the chain $\text{CIM} \rightarrow \text{NCCM} \rightarrow \text{ECCM}$ in even their truncated versions, leads to the possibility of an increasing degree of effective compactification of the phase space. In turn one might hope that this should allow the physically important region for any particular application to be described in terms of an effective mean field theory of reduced dimensionality, and which for the ECCM is completely multilocal in character.

The CC techniques have already been very successfully applied to a wide range of physical systems in quantum chemistry [12, 15, 20–22], condensed matter physics [23–25], nuclear physics [10, 14, 26, 27], and to various model problems of interest in quantum field theory [28–34]. Furthermore, since in the ECCM (and only in the ECCM) *all* of the basic amplitudes obey the exact cluster property, this parametrization is capable in principle of describing such phenomena as phase transitions, states of topological excitation or deformation, and spontaneous symmetry breaking. Particular applications to date have included gauge-field descriptions of both a charged impurity in a polarizable medium [35] (of relevance, for example, to the important experimental tool of positron annihilation in metals) and the zero-temperature hydrodynamics of a strongly-interacting condensed Bose fluid [36].

In view of the considerable theoretical advantages outlined above of the various

IC parametrization schemes, and their potential applicability to other more intractable problems in quantum field theory, it is clearly of fundamental interest to examine carefully such basic features as their existence and convergence properties [37]. Furthermore, such concepts as the connectivity and multiple linking properties of the subsystem amplitudes and the associated topology of the emergent tree-diagram structures in the various IC parametrizations have mostly been analyzed diagrammatically in the past [13]. It is clear that the precise meaning of such diagrammatic expansions can only properly be established in the light of their convergence properties. The main aim of the present work is to present a unified *algebraic* description of each of the IC parametrizations and their underlying features, so that the above concepts can be studied as rigorously as possible.

In order to carry out this aim it is convenient to choose in the first place a model field theory which, on the one hand, is sufficiently simple to be able to implement as fully as possible. On the other hand, it should be highly nontrivial to handle by alternative many-body means, and it should also provide a stringent test of the IC techniques. Ideal in this respect is the class of one-body Schrödinger problems in one dimension, considered as the corresponding one-mode bosonic field theories characterized by a single one-body creation operator $a^\dagger$, and its Hermitian adjoint destruction counterpart, a . Such problems are just the $(0+1)$ -dimensional analogues of real field theories in a nonzero number of space dimensions. When necessary to choose a specific interaction potential, we may also consider the various anharmonic oscillator (AO) models. Such models are well known to fail to converge in perturbation theory for *any* strength of the anharmonic potential [38–40]. Furthermore, all such models are highly singular in the sense of exhibiting maximal nonlocality, and hence they are expected to be a severe test for the CC techniques in particular, which are specifically geared towards local field theories or systems with normal locality and separability properties.

Finally, a particularly useful way to implement our aim to algebraize our model is to consider its holomorphic representation in which the original bosonic field theory is mapped into a classical field theory for a corresponding function of the complex variable z in the well-known Bargmann Hilbert space [41–42]. This space is characterized by one of various possible specific forms for the inner product between two complex functions. These forms are identical in the usual case where the space is restricted to normalizable states. In the present paper we discuss in detail the holomorphic representations of the various operators that characterize each of the three IC parametrizations. One of our main findings is that the NCCM and ECCM representations actually necessitate extending the Hilbert space of normalizable wave functions to a more general linear vector space. Formally divergent series thereby arise. Nevertheless, we are able to show how these may be regularized to obtain precise, but generally nonunique, interpretations such that the expectation values for arbitrary operators are well defined.

The outline of the remainder of the paper is as follows. In Section II we first describe in very general terms the key features of the three IC parametrizations that we have already alluded to above. We then discuss in Section III the properties of

the holomorphic wave functions for the ground states of the one-dimensional Schrödinger problems considered, using the AO systems as a specific model. The resulting Bargmann-space representation of the CIM functions and amplitudes is extended in Section IV to their counterparts for both the NCCM and ECCM. After describing in Section V how general expectation values of arbitrary operators may be derived in a wholly algebraic fashion via a specific CC generating functional, the results are summarized and discussed in Section VI. In particular, we emphasize how the states generated by the CC parametrizations may also profitably be viewed as multicoherent or supercoherent states in the sense that the usual Glauber (or one-boson) coherent states which fundamentally underpin the holomorphic representation, may be extended to squeezed (or two-boson) coherent states (and see Appendix A), and thence to the “hypersqueezed” or (n -boson, with $n > 2$) multicoherent states.

In a subsequent paper (II) we shall focus attention on the classical Hamiltonian and on the structure of the phase space induced by each of the IC parametrizations. We further discuss there the diagrammatic interpretation of the various IC methods in terms of the associated tree diagrams.

II. BASIC ELEMENTS OF THE VARIOUS INDEPENDENT-CLUSTER PARAMETRIZATIONS

We consider the general time-dependent Schrödinger equations for the exact ket states $|\psi\rangle = |\psi(t)\rangle$ and bra states $\langle\tilde{\psi}| = \langle\tilde{\psi}(t)|$ of an arbitrary many-body system,

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

which exist within the many-body Hilbert space $\mathcal{H}$. It is convenient to choose the normalization such that $\langle\tilde{\psi}|\psi\rangle = 1$ for all times t , so that when the Hamiltonian H is Hermitian, as usual, $H = H^\dagger$, we have $\langle\tilde{\psi}| = \langle\psi|\psi\rangle^{-1}\langle\psi|$, with $\langle\psi| = (|\psi\rangle)^\dagger$.

For ease of presentation we restrict ourselves to “closed-shell” (or non-degenerate) systems, so that the exact states of the system may sensibly be referred to some suitably chosen *single* model (or reference) state, denoted as $|0\rangle$. The choice of this state $|0\rangle$ is rather free, provided only that it satisfies the role of a *cyclic vector*, in the sense that the algebra of all possible operators in $\mathcal{H}$ is spanned by the two Abelian subalgebras of creation and destruction operators defined with respect to it. In this way we may define suitable complete orthonormal sets of configuration creation operators $\{C_I^\dagger\}$ and their Hermitian adjoint counterparts $\{C_I\}$. Each many-body configuration-space index I represents some appropriate *set* of (discrete or continuous) single-particle labels which are chosen to distinguish the one-particle modes within the theory. Each index I thus defines a subsystem or cluster within the full system, of a given configuration. Our only assumption is that the creation and destruction subalgebras and the state $|0\rangle$ are cyclic in the sense

that all of the ket states in $\mathcal{H}$ can be constructed from linear combinations of states $\{C_I^\dagger |0\rangle\}$; and similarly for the bra states with respect to the states $\{\langle 0| C_I\}$. The total description is *bicommutative* in the sense that both subalgebras are assumed to be Abelian.

The actual choice of the configuration set-indices $\{I\}$ clearly depends upon the particular system under consideration. Examples have been given elsewhere [16]. For present purposes, the only properties that we require are: (i) orthonormality,

$$\langle 0| C_I C_J^\dagger |0\rangle = \delta(I, J), \quad (2.2)$$

where $\delta(I, J)$ is an appropriately defined Kronecker symbol; and (ii) completeness, which implies the resolution of the identity operator $\mathbb{1}$ within $\mathcal{H}$,

$$\begin{aligned} \mathbb{1} &= \sum_I C_I^\dagger |0\rangle \langle 0| C_I \\ &\equiv |0\rangle \langle 0| + \sum_I' C_I^\dagger |0\rangle \langle 0| C_I, \end{aligned} \quad (2.3)$$

where the prime on a sum over configurations here and henceforth restricts us to excluding the null configuration $I=0$, with $C_0^\dagger = \mathbb{1} = C_0$. Each of our three IC parametrizations is now specified in terms of the above configurations.

In order to do this it is convenient to introduce first the action functional,

$$\mathcal{A} \equiv \int_{t_1}^{t_2} dt \langle \tilde{\psi}(t) | (i\partial/\partial t - H) | \psi(t) \rangle, \quad (2.4)$$

in terms of which Eqs. (2.1) are completely equivalent to the stationarity principle,

$$\delta \mathcal{A} / \delta \langle \tilde{\psi} | = 0 = \delta \mathcal{A} / \delta | \psi \rangle, \quad (2.5)$$

for all independent variations in the bra and ket states such that $|\delta \psi(t_j)\rangle = 0 = \langle \delta \tilde{\psi}(t_j) |$; $j=1, 2$. Different parametrizations of the bra and ket states now lead to different implementations of this variational principle. The simplest is certainly the CIM parametrization, defined as

$$\begin{aligned} | \psi \rangle &= F | 0 \rangle; & \langle \tilde{\psi} | &= \langle 0 | \tilde{F}, \\ F &= \sum_I f_I C_I^\dagger; & \tilde{F} &= \sum_I \tilde{f}_I C_I, \end{aligned} \quad (2.6)$$

which does not yet manifestly satisfy the normalization condition $\langle \tilde{\psi} | \psi \rangle = 1$, but from which it is trivial to show that Eq. (2.5) leads to the canonical equations of motion,

$$i \frac{df_I}{dt} = \frac{\partial \bar{H}}{\partial \tilde{f}_I}; \quad -i \frac{d\tilde{f}_I}{dt} = \frac{\partial \bar{H}}{\partial f_I}, \quad (2.7)$$

in terms of the energy expectation value $\bar{H} \equiv \langle \tilde{\psi}(t) | H | \psi(t) \rangle \equiv \bar{H}[f_I, \tilde{f}_I; t]$. Equations (2.7) are exact provided that the configuration space is not truncated. Conversely, if the sums in Eq. (2.6) are approximated to run over only a selected number of configurations, Eqs. (2.7) become the standard approximate CIM (or time-dependent generalized shell model) equations.

The great advantage of the CIM parametrization is its simplicity. Nevertheless, the multiplicative separability property of the wave function in the limit that the system dissociates into two non-interacting fragments, is clearly not incorporated in the parametrization of Eq. (2.6) when the sums over configurations are truncated, as would be necessary in practice. It is this feature which leads to the CIM not satisfying the closely related requirements of size-consistency [18, 43] and size-extensivity [18, 44] at finite levels of truncation and which hence makes the method unusable in principle for extended systems and computationally problematical in practice for large systems. In the NCCM parametrization,

$$\begin{aligned} |\psi\rangle &= k e^S |0\rangle; & \langle\tilde{\psi}| &= \frac{1}{k} \langle 0| \tilde{S} e^{-S}, \\ S &= \sum_I s_I C_I^\dagger; & \tilde{S} &= 1 + \sum_I \tilde{s}_I C_I, \end{aligned} \quad (2.8)$$

in which the normalization condition $\langle\tilde{\psi}|\psi\rangle = 1$ is explicit, and where $k = k(t)$ is a time-dependent c-number scale factor, this problem is cured for the ket states. Thus the multiplicative separability of the exact wave operator F is now reflected in the additive separability of the cluster operator $S = S(t)$, and is exactly preserved even when the sum over configurations for S in Eq. (2.8) is truncated.

On the other hand, the bra states still do not separate properly in the dissociation limits, because the operator $\tilde{S}$ still needs to be multiplicatively separable, which is again violated upon truncating the sum over configurations for $\tilde{S}$ in Eq. (2.8). Nevertheless, there is a compelling reason to parametrize the bra and ket states in the NCCM in this seemingly rather asymmetrical fashion which, furthermore, does not manifestly preserve their Hermitian conjugacy. This form does, however, preserve the canonical form of the equations of motion (2.7) in the following sense. Thus, if we write these generically as,

$$i \frac{dx_I}{dt} = \frac{\partial \bar{H}}{\partial \tilde{x}_I}; \quad -i \frac{d\tilde{x}_I}{dt} = \frac{\partial \bar{H}}{\partial x_I}, \quad (2.9)$$

with $\bar{H} \equiv \langle \tilde{\psi}(t) | H | \psi(t) \rangle \equiv \bar{H}[x_I, \tilde{x}_I; t]$, then the NCCM parametrization of Eq. (2.8) is also easily seen from Eq. (2.4) to satisfy Eq. (2.9) with $\{x_I, \tilde{x}_I\} \rightarrow \{s_I, \tilde{s}_I\}$ in exactly the same way that the CIM also does with $\{x_I, \tilde{x}_I\} \rightarrow \{f_I, \tilde{f}_I\}$, although the NCCM functional form of the energy expectation value $\bar{H}[s_I, \tilde{s}_I; t]$ will be quite different from the CIM functional form $\bar{H}[f_I, \tilde{f}_I; t]$.

Finally, the separability of the NCCM bra-state wave functions can easily be

guaranteed at a stroke by similarly rewriting the correlation operator $\tilde{S}$ in the (linked-cluster) exponential form,

$$\tilde{S} \equiv \exp(\tilde{\Sigma}), \quad (2.10)$$

which now characterizes the ECCM. Although the ECCM may be fully specified in terms of the operators $\{S, \tilde{S}\}$, it is clear that these cannot form a canonically conjugate pair in the sense that their amplitudes obey Eq. (2.9). On the other hand, it is a simple matter to verify that if the ECCM is instead specified in terms of the operators $\{\Sigma, \tilde{\Sigma}\}$ defined as

$$\begin{aligned} |\psi\rangle &= k e^S |0\rangle; & \langle\tilde{\psi}| &= \frac{1}{k} \langle 0| e^{\tilde{S}} e^{-S}, \\ \Sigma |0\rangle &= Q e^{\tilde{S}} S |0\rangle; & Q &\equiv 1 - |0\rangle\langle 0|, \\ \Sigma &= \sum_I' \sigma_I C_I^\dagger; & \tilde{\Sigma} &= \sum_I' \tilde{\sigma}_I C_I, \end{aligned} \quad (2.11)$$

then the ECCM amplitudes $\{x_I \rightarrow \sigma_I, \tilde{x}_I \rightarrow \tilde{\sigma}_I\}$ also satisfy the canonical equations of motion (2.9). It is easily seen that the inverse relationships between the ECCM amplitudes $\{\sigma_I\}$ and their NCCM counterparts $\{s_I\}$ are given by

$$\sigma_I = \langle 0| C_I \tilde{S} S |0\rangle; \quad s_I = \langle 0| C_I e^{-\tilde{\Sigma}} \Sigma |0\rangle, \quad (2.12)$$

and hence that either of the sets $\{s_I, \tilde{\sigma}_I\}$ or $\{\sigma_I, \tilde{s}_I\}$ is complete and sufficient to specify the ECCM parametrization. It is clear from Eq. (2.12) that the amplitudes $\{\sigma_I\}$ are also linked-cluster amplitudes, given that the amplitudes $\{s_I\}$ are.

So far we have discussed the dynamical behaviour of the system. The exact stationary ground-state energy eigenvalue E_0 and eigenfunctions $|\psi_0\rangle$ and $\langle\tilde{\psi}_0|$,

$$H |\psi_0\rangle = E_0 |\psi_0\rangle; \quad \langle\tilde{\psi}_0| H = E_0 \langle\tilde{\psi}_0|, \quad (2.13)$$

are similarly found by requiring the exact energy expectation value, $\bar{H} \equiv \bar{H}[x_I, \tilde{x}_I] \equiv \langle\tilde{\psi}| H |\psi\rangle$ to be stationary,

$$\frac{\partial \bar{H}}{\partial x_I} = 0 = \frac{\partial \bar{H}}{\partial \tilde{x}_I}, \quad (2.14)$$

subject to the normalization constraint, $\langle\tilde{\psi}|\psi\rangle = 1$. In the NCCM and ECCM parametrizations this constraint is made manifest from the outset by the choice $k \rightarrow 1$ in Eqs. (2.8) and (2.11) for the time-independent situation, and hence only non-null configurations, $I \neq 0$, enter into Eq. (2.14). In such cases the time-independent ket state $|\psi\rangle$ then also satisfies the intermediate normalization, $\langle 0|\psi\rangle = 1$, from Eq. (2.8), which further implies that $f_0 = 1$ within the CIM parametrization of Eq. (2.6). We note that although all three ground-state IC methods have been cast as the variational equations (2.14), the resulting estimates for E_0 when the full

space $\mathcal{H}$ is restricted to a subset of configurations from the full set $\{I\}$, are not necessarily upper bounds to the exact ground-state energy. Thus, the quantity $\langle \tilde{\psi} | (H - E_0) | \psi \rangle / \langle \tilde{\psi} | \psi \rangle$ is only manifestly non-negative for all wave functions $\langle \tilde{\psi} |$ and $|\psi\rangle$ when $\langle \tilde{\psi} | \propto (|\psi\rangle)^\dagger$. While this explicit Hermitian conjugacy holds in the CIM at all levels of truncation, it does not generally hold true for the truncated NCCM and ECCM parametrizations.

Excited states of the system may also be investigated in all three IC parametrizations by considering the dynamics of small oscillations around the above equilibrium time-independent ground-state values $\{x_I^0, \tilde{x}_I^0\}$, which are obtained as the solution to the variational equations (2.14), subject to the normalization condition $\langle \tilde{\psi} | \psi \rangle = 1$. If we write $x_I(t) \rightarrow x_I^0 + \delta x_I(t)$, $\tilde{x}_I(t) \rightarrow \tilde{x}_I^0 + \delta \tilde{x}_I(t)$, then close to the stationary ground state the energy expectation value becomes

$$\bar{H} \rightarrow \bar{H}^{(2)} = E_0 + \sum_I \sum_J (\delta \tilde{x}_I \mathcal{E}_{IJ} \delta x_J + \frac{1}{2} \delta \tilde{x}_I \tilde{\mathcal{F}}_{IJ} \delta \tilde{x}_J + \frac{1}{2} \delta x_I \mathcal{F}_{IJ} \delta x_J), \quad (2.15)$$

including terms up to second order only, and where $E_0 \equiv \bar{H}[x_I^0, \tilde{x}_I^0]$ and $\mathcal{E}_{IJ}$, $\mathcal{F}_{IJ}$, and $\tilde{\mathcal{F}}_{IJ}$ are the second-order partial derivatives of $\bar{H}$,

$$\mathcal{E}_{IJ} = \left. \frac{\partial^2 \bar{H}}{\partial \tilde{x}_I \partial x_J} \right|_0; \quad \mathcal{F}_{IJ} = \left. \frac{\partial^2 \bar{H}}{\partial x_I \partial x_J} \right|_0; \quad \tilde{\mathcal{F}}_{IJ} = \left. \frac{\partial^2 \bar{H}}{\partial \tilde{x}_I \partial \tilde{x}_J} \right|_0, \quad (2.16)$$

evaluated at the stationary point $\{x_I^0, \tilde{x}_I^0\}$. From Eq. (2.9), the dynamical linear response equations can thus be written in block matrix form,

$$i \frac{d}{dt} \begin{pmatrix} \delta x_I \\ \delta \tilde{x}_I \end{pmatrix} = \sum_J \begin{pmatrix} \mathcal{E}_{IJ} & \tilde{\mathcal{F}}_{IJ} \\ -\mathcal{F}_{IJ} & -\mathcal{E}_{JI} \end{pmatrix} \begin{pmatrix} \delta x_J \\ \delta \tilde{x}_J \end{pmatrix}. \quad (2.17)$$

Equation (2.17) is just a classical normal modes problem. By seeking solutions for δx_I and $\delta \tilde{x}_I$ proportional to $\exp(-i\epsilon t)$, the eigenfrequencies $\{\epsilon\}$ are simply seen to be obtained by diagonalizing the effective Hamiltonian H_D , which can be written in an obvious block matrix notation as,

$$H_D \equiv \begin{pmatrix} \mathcal{E} & \tilde{\mathcal{F}} \\ -\mathcal{F} & -\mathcal{E}^T \end{pmatrix} = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} \begin{pmatrix} \mathcal{F} & \mathcal{E}^T \\ \mathcal{E} & \tilde{\mathcal{F}} \end{pmatrix}, \quad (2.18)$$

where the superscript T on a matrix indicates its transpose. Since both $\mathcal{F}$ and $\tilde{\mathcal{F}}$ are symmetric matrices from their defining equation (2.16), the product form for H_D in Eq. (2.18) shows that H_D is a product of an antisymmetric with a symmetric matrix. A general theorem [45] then shows that the eigenvalues $\{\epsilon\}$ appear in pairs $\epsilon = \pm \epsilon_\lambda$. The set $\{\epsilon_\lambda\}$ are just the excitation energy eigenvalues (i.e., measured with respect to E_0) [17].

It is also clear that the equation of motion for the expectation value $\bar{A} \equiv \langle \tilde{\psi}(t) | A(t) | \psi(t) \rangle \equiv \bar{A}[x_I, \tilde{x}_I; t]$ of an arbitrary operator $A = A(t)$ in $\mathcal{H}$, can be specified as

$$\frac{d\bar{A}}{dt} = \frac{\partial \bar{A}}{\partial t} + \sum_I \left(\frac{\partial \bar{A}}{\partial x_I} \frac{dx_I}{dt} + \frac{\partial \bar{A}}{\partial \tilde{x}_I} \frac{d\tilde{x}_I}{dt} \right). \quad (2.19)$$

This can be rewritten using the classical Hamiltonian equations of motion (2.9) in the form

$$\frac{d\bar{A}}{dt} = \frac{\partial \bar{A}}{\partial t} + \{\bar{A}, \bar{H}\}, \quad (2.20)$$

in terms of the (generalized) classical Poisson bracket, defined between the expectation values $\bar{A}$ and $\bar{B}$ of two arbitrary operators A and B in $\mathcal{H}$ as

$$\{\bar{A}, \bar{B}\} = \frac{1}{i} \sum_I \left(\frac{\partial \bar{A}}{\partial x_I} \frac{\partial \bar{B}}{\partial \tilde{x}_I} - \frac{\partial \bar{A}}{\partial \tilde{x}_I} \frac{\partial \bar{B}}{\partial x_I} \right). \quad (2.21)$$

In terms of the “fields” $\{\phi_I\}$ and their canonically conjugate “momentum densities” $\{\pi_I\}$, defined as

$$\phi_I = 2^{-1/2}(x_I + \tilde{x}_I); \quad \pi_I = 2^{-1/2}i(\tilde{x}_I - x_I), \quad (2.22)$$

Eq. (2.21) has the even more standard form,

$$\{\bar{A}, \bar{B}\} = \sum_I \left(\frac{\partial \bar{A}}{\partial \phi_I} \frac{\partial \bar{B}}{\partial \pi_I} - \frac{\partial \bar{A}}{\partial \pi_I} \frac{\partial \bar{B}}{\partial \phi_I} \right). \quad (2.23)$$

The phase space $\{\phi_I, \pi_I\}$ for each IC parametrization clearly has the canonical symplectic structure

$$\begin{aligned} \{\phi_I, \pi_J\} &= \delta(I, J), \\ \{\phi_I, \phi_J\} &= 0 = \{\pi_I, \pi_J\}. \end{aligned} \quad (2.24)$$

Equation (2.20) is clearly the classical, exactly mapped version of the usual quantum-mechanical Heisenberg equation of motion for the operator A in the original Hilbert space $\mathcal{H}$,

$$\frac{dA}{dt} = \frac{\partial A}{\partial t} + \frac{1}{i} [A, H], \quad (2.25)$$

and it is valid in all three IC parametrizations.

Finally, it is possible to show that the expectation value of an arbitrary commutator between *any* two operators A and B in $\mathcal{H}$ is also exactly mapped by each

IC parametrization into the corresponding Poisson bracket of Eq. (2.21) or Eq. (2.23),

$$\langle \tilde{\psi} | [A, B] | \psi \rangle = i \{ \bar{A}, \bar{B} \}. \quad (2.26)$$

This relation is straightforward to prove for the CIM parametrization, but is by no means trivial for the two CC parametrizations. For the CIM we have

$$\begin{aligned} \langle \tilde{\psi} | AB | \psi \rangle &= \langle 0 | \tilde{F}ABF | 0 \rangle \\ &= \sum_I \langle 0 | \tilde{F}AC_I^\dagger | 0 \rangle \langle 0 | C_I BF | 0 \rangle, \end{aligned}$$

where we have inserted a resolution of the identity operator from Eq. (2.3). We thus immediately have the result

$$\langle \tilde{\psi} | AB | \psi \rangle = \sum_I \frac{\partial \bar{A}}{\partial f_I} \frac{\partial \bar{B}}{\partial \tilde{f}_I}, \quad (2.27)$$

and hence also the relation (2.26) for the CIM parametrization.

In the case of the NCCM we similarly have

$$\begin{aligned} \langle \tilde{\psi} | AB | \psi \rangle &= \langle 0 | \tilde{S}e^{-S}ABe^S | 0 \rangle \\ &= \sum_I \langle 0 | \tilde{S}e^{-S}Ae^SC_I^\dagger | 0 \rangle \langle 0 | C_I e^{-S}Be^S | 0 \rangle. \end{aligned} \quad (2.28)$$

We may also readily derive the relations

$$\begin{aligned} \frac{\partial \bar{A}}{\partial s_I} &= \langle 0 | \tilde{S}e^{-S}[A, C_I^\dagger]e^S | 0 \rangle, \\ \frac{\partial \bar{B}}{\partial \tilde{s}_I} &= \langle 0 | C_I e^{-S}Be^S | 0 \rangle. \end{aligned} \quad (2.29)$$

Recalling that $[S, C_I^\dagger] = 0$, and using Eqs. (2.28) and (2.29), we find

$$\begin{aligned} \langle \tilde{\psi} | AB | \psi \rangle &= \sum_I' \frac{\partial \bar{A}}{\partial s_I} \frac{\partial \bar{B}}{\partial \tilde{s}_I} + \sum_I \langle 0 | \tilde{S}C_I^\dagger e^{-S}Ae^S | 0 \rangle \langle 0 | C_I e^{-S}Be^S | 0 \rangle \\ &= \sum_I' \frac{\partial \bar{A}}{\partial s_I} \frac{\partial \bar{B}}{\partial \tilde{s}_I} + \sum_I \sum_J \langle 0 | \tilde{S}C_I^\dagger C_J^\dagger | 0 \rangle \langle 0 | C_J e^{-S}Ae^S | 0 \rangle \\ &\quad \times \langle 0 | C_I e^{-S}Be^S | 0 \rangle. \end{aligned} \quad (2.30)$$

The last term in Eq. (2.30) is clearly symmetric under the interchange of A and B , since $[C_I^\dagger, C_J^\dagger] = 0$, and thus the relation (2.26) immediately follows for the NCCM parametrization. The proof of Eq. (2.26) for the ECCM case is similar but slightly more tedious, and we do not therefore give it here.

To summarize so far, we have seen how each of the three IC parametrizations, namely, (i) the CIM, (ii) the NCCM, and (iii) the ECCM, satisfies both the dynamical equation of motion (2.1) and the time-independent ground-state equation (2.13) in $\mathcal{H}$, in the same generic canonical form of Eq. (2.9) and its static counterpart of Eq. (2.14), respectively. The canonically conjugate fundamental operators $\{X, \tilde{X}\}$ are respectively (i) $\{F, \tilde{F}\}$, (ii) $\{S, \tilde{S}\}$, and (iii) $\{\Sigma, \tilde{\Sigma}\}$. Only in the case of the CIM are the resulting equations linear. Both CC parametrizations provide intrinsically nonlinear decompositions of the underlying Schrödinger equation (2.1) or (2.13). In each IC method the parametrized equations of motion (2.9) are just the classical canonical equations in a (multi-body) phase space wherein the canonical coordinates are just the multiconfigurational correlation amplitudes $\{x_I, \tilde{x}_I\}$ themselves. The structure of the phase space in each case is that of a complex differentiable manifold with a symplectic structure induced by a generalized classical Poisson bracket form between the amplitudes. Diagonalizing the effective Hamiltonian which governs small oscillations around the equilibrium ground state is equivalent to performing a canonical coordinate transformation (i.e., a symplectomorphism) into normal coordinates in the symplectic phase space. The normal frequencies are just the excitation energies.

Although the three corresponding IC classical phase spaces, parametrized and spanned by the respective sets of coordinates $\{x_I, \tilde{x}_I\}$ are in principle of equal complexity, the three separate forms of the Hamiltonian functional $\bar{H}[x_I, \tilde{x}_I; t]$ lead to distinct differences. These differences are a reflection of the underlying separability and locality properties of the three methods. Whereas the exact wave operators F and $\tilde{F}$ and the correlation operator $\tilde{S}$ are multiplicatively separable, the various cluster operators S, Σ , and $\tilde{\Sigma}$ are additively separable. The important physical properties of extended systems are extensive quantities. These are obviously most directly formulated in terms of parameters which are additively separable even when the complete description is approximated by truncating the multiconfigurational phase space.

We note parenthetically that all three IC methods can thus be systematically approximated. One common such approximation scheme is the so-called SUB(n) truncation scheme in which only configurations described by indices I for the amplitudes $\{x_I, \tilde{x}_I\}$ containing up to n -tuple excitations (e.g., of single particles for bosonic systems with the bare vacuum as model state $|0\rangle$, or particle-hole pairs for fermionic systems with a filled Fermi sea model state $|0\rangle$) are included in the sums over configurations. In all three parametrizations this results in finite expressions for $\bar{H} = \bar{H}[x_I, \tilde{x}_I; t]$ at all SUB(n) levels.

The separability and locality properties of the various IC parametrizations are in turn intrinsically related to the connectivity properties of the respective sets of amplitudes $\{x_I, \tilde{x}_I\}$. The equilibrium NCCM coefficients $\{s_I^0\}$, for example, are just the Hubbard linked-cluster amplitudes which represent the sums of complete sets of connected (or linked) open-ended Goldstone diagrams for the ground state. By contrast, the CIM amplitudes $\{f_I^0\}$ also contain disconnected (or unlinked) terms. Indeed, all of the amplitudes $\{s_I\}$, $\{\sigma_I\}$, and $\{\tilde{\sigma}_I\}$ are linked, whereas the

amplitudes $\{f_I\}$, $\{\tilde{f}_I\}$, and $\{\tilde{s}_I\}$ contain unlinked terms. In particular, of the three IC parametrizations, the ECCM is the only one in which all of the amplitudes are fully linked and hence multilocal in the sense of obeying the cluster property in the coordinate-space representation. The various connectivity properties of the three parametrizations are also intimately related to the various "generalized time ordering" properties [13] associated with the generalized tree diagram structures which emerge from each method in connection with the (time-independent perturbation theory) expansions for arbitrary expectation values $\bar{A} = \bar{A}[x_I^0, \tilde{x}_I^0]$. These diagrammatic and topological aspects of the various IC parametrizations are considered further in a subsequent paper II.

Despite the obvious intuitive appeal of the ECCM in particular, many open questions remain. We have seen how it provides in principle an exact mapping of linear quantum mechanics into an equivalent but highly nonlinear classical mechanics. On the other hand, the actual existence of the ECCM phase space for infinite Hilbert spaces $\mathcal{H}$ is by no means obvious. The related problem of the convergence properties of the method and the associated need for any appropriate regularization procedures, are clearly fundamental in this regard. In order to begin to address such questions we turn now in Section III to the particular class of one-mode bosonic field theories as a stringent model test case.

III. HOLOMORPHIC WAVE FUNCTIONS FOR THE GROUND STATES OF ONE-DIMENSIONAL ANHARMONIC OSCILLATOR SYSTEMS

The Hamiltonian H for a one-body Schrödinger problem in one space dimension $x \in (-\infty, \infty)$,

$$H = \frac{1}{2} \hat{p}^2 + V(\sqrt{2} \hat{x}), \quad (3.1)$$

may readily be construed as single-mode (or $(0+1)$ -dimensional) bosonic field theory. Thus, the position operator $\hat{x}$ ($\rightarrow x$) and the conjugate momentum operator $\hat{p}$ ($\rightarrow -id/dx$) are mapped into their canonical Fock-space creation and destruction counterparts, $a^\dagger$ and a , respectively,

$$\hat{x} = 2^{-1/2}(a^\dagger + a); \quad \hat{p} = 2^{-1/2}i(a^\dagger - a), \quad (3.2)$$

which hence obey the usual bosonic canonical commutation relations (CCR),

$$[a, a^\dagger] = 1. \quad (3.3)$$

The Fock-space counterpart to Eq. (3.1) is thus

$$H = -\frac{1}{4}(a^\dagger - a)^2 + V(a^\dagger + a). \quad (3.4)$$

A convenient choice for the (normalized) model state or cyclic vector $|0\rangle$ for the

model field theory of Eq. (3.4) is clearly the ground state of the harmonic oscillator Hamiltonian,

$$H^0 = \frac{1}{2} \hat{p}^2 + \frac{1}{2} \hat{x}^2 = a^\dagger a + \frac{1}{2}, \quad (3.5)$$

which satisfies the usual role of the vacuum state,

$$a |0\rangle = 0. \quad (3.6)$$

Its coordinate-space representation is given as

$$\langle x|0\rangle \equiv \phi(x) = \pi^{-1/4} \exp(-\frac{1}{2}x^2); \quad \langle 0|0\rangle = 1. \quad (3.7)$$

For these single-mode field theories, the role of the (orthonormal) configuration-space creation operators $C_I^\dagger$ is simply played by the n -boson creation operators, $C_I^\dagger \rightarrow (n!)^{-1/2} (a^\dagger)^n$,

$$\langle 0| a^m (a^\dagger)^n |0\rangle = n! \delta_{mn}, \quad (3.8)$$

and the general set-index I is replaced by the single integer n . For present purposes it is actually more convenient to treat the (unnormalized) operators $(a^\dagger)^n$ as the basic configurational creation operators, and hence to modify the general normalization convention used in Eq. (2.2) to that implied by Eq. (3.8). Arbitrary ket and bra states in the Fock space can now be represented in the form

$$\begin{aligned} |g\rangle &\equiv g(a^\dagger) |0\rangle; & \langle f^*| &\equiv \langle 0| f(a) = (f^*(a^\dagger) |0\rangle)^\dagger = (|f^*\rangle)^\dagger, \\ g(z) &\equiv \sum_{n=0}^{\infty} g_n z^n; & f(z) &\equiv \sum_{n=0}^{\infty} f_n z^n. \end{aligned} \quad (3.9)$$

Use of Eq. (3.8) now yields the scalar product of two such states as

$$\langle 0| f(a) g(a^\dagger) |0\rangle = \langle f^*|g\rangle = \sum_{n=0}^{\infty} n! f_n g_n, \quad (3.10)$$

and the assumption that the states are normalizable assures that the sum in Eq. (3.10) is convergent. It is also immediately clear that equivalent ways of writing Eq. (3.10) are the alternative forms,

$$\langle f^*|g\rangle = f(d/dz) g(z)|_{z=0} = g(d/dz) f(z)|_{z=0}. \quad (3.11)$$

Finally, we may make use of the elementary integral over the complex plane

$$\int d^2z z^m z^{*n} \exp(-|z|^2) = \pi n! \delta_{mn} \quad (3.12)$$

to write the scalar product in the final forms

$$\begin{aligned}\langle f^* | g \rangle &= \frac{1}{\pi} \int d^2z \, e^{-|z|^2} f(z) g(z^*) \\ &= \frac{1}{\pi} \int d^2z \, e^{-|z|^2} f(z^*) g(z).\end{aligned}\quad (3.13)$$

It is clear that the normalizability of the states $|g\rangle$ and $\langle f^*|$ is reflected via Eq. (3.13) in the requirement that both (holomorphic) functions $f(z)$ and $g(z)$ must be entire functions of order $\rho \leq 2$ (and type $\tau \leq \frac{1}{2}$, if $\rho = 2$). In this case, each of the three relations (3.10), (3.11), and (3.13) yields identical (convergent) results. The space of such functions is denoted as the Bargmann Hilbert space [41, 42], and the corresponding representation of the wave functions as the holomorphic (or Bargmann) representation. In the Bargmann space the CCR algebra is represented directly by the algebra

$$a^\dagger \rightarrow z; \quad a \rightarrow \frac{d}{dz} \quad (3.14)$$

of the complex variable z and its derivative. A very natural role is now played by the usual Glauber coherent states $|z\rangle$, which are the (normalized) eigenstates of the fundamental destruction operator a ,

$$a |z\rangle = z |z\rangle; \quad \langle z| a^\dagger = z^* \langle z|. \quad (3.15)$$

The explicit construction of these states and various useful properties of them, are summarized in Appendix A. For example, the form (3.13) of the inner product can be derived directly by insertion of the resolution (A8) of the identity operator in terms of this overcomplete set of states

$$\begin{aligned}\langle f^* | g \rangle &= \frac{1}{\pi} \int d^2z \, \langle 0| f(a) |z\rangle \langle z| g(a^\dagger) |0\rangle \\ &= \frac{1}{\pi} \int d^2z \, f(z) g(z^*) |\langle 0|z\rangle|^2,\end{aligned}\quad (3.16)$$

and where in the second equality we have used the fundamental relation (3.15). Use of the overlap relation (A7) then immediately shows the equivalence of Eqs. (3.13) and (3.16).

Arbitrary states in the Fock space now have the equivalent holomorphic representations

$$\begin{aligned}g(a) f(a^\dagger) |0\rangle &\equiv h(a^\dagger) |0\rangle \leftrightarrow g(d/dz) f(z) = h(z) \\ \langle 0| g(a) f(a^\dagger) &\equiv \langle 0| \tilde{h}(a) \leftrightarrow f(d/dz) g(z) = \tilde{h}(z).\end{aligned}\quad (3.17)$$

Equations (3.17) also immediately imply the alternative forms (3.11) of the inner product. In this way our bosonic quantum field theory in the Fock space may be mapped into the corresponding (classical) field theory of a complex function in the normed Bargmann space. The ground-state Schrödinger equation (2.13) with the Hamiltonian of Eq. (3.1), or equivalently Eq. (3.4), becomes the ordinary differential equation in the complex plane,

$$-\frac{1}{4}(d/dz - z)^2 F^0(z) + V(d/dz + z) F^0(z) = E_0 F^0(z), \quad (3.18)$$

in terms of the CIM representation,

$$|\psi_0\rangle = F^0(a^\dagger) |0\rangle, \quad (3.19)$$

of the ground-state wave function. By writing $F^0(z)$ in the form

$$F^0(z) \equiv \exp(-\frac{1}{2}z^2) f^0(z), \quad (3.20)$$

Eq. (3.18) can also be written in the equivalent form,

$$-\left(\frac{1}{2} \frac{d}{dz} - z\right)^2 f^0(z) + V(d/dz) f^0(z) = E_0 f^0(z). \quad (3.21)$$

We have seen in Section II how the wave functions in the original Schrödinger Hilbert space $\mathcal{H}$ or the equivalent bosonic Fock space may be parametrized in terms of the fundamental operators $\{X, \tilde{X}\}$ for each of the three IC cases. The corresponding configuration-space amplitudes $\{x_I, \tilde{x}_I\}$ may clearly be associated with respective ket and bra states $X|0\rangle$ and $\langle 0|\tilde{X}$, although we stress that only in the CIM case are these states necessarily physical in the sense of definitely belonging to $\mathcal{H}$. Nevertheless, such (fictitious) states may also be introduced for the two CC parametrizations, and we shall see in Section IV that they play an almost indispensable intermediate role in practice. Indeed, inspection of Eqs. (2.11) and (2.8), for example, shows that it is tempting to regard the states $S|0\rangle$ and $\langle 0|\tilde{S}$ as having an independent existence. We shall show explicitly in Section IV, however, that neither of these states is generally normalizable. Their introduction therefore can cause serious problems of interpretation. This typically manifests itself by the appearance of formally divergent sums or integrals.

For example, although each of the relations (3.10), (3.11), and (3.13) for the inner product of two wave functions in $\mathcal{H}$ yields identical convergent results for normalizable states, differences can certainly arise when the space $\mathcal{H}$ of allowable wave functions is extended to a more general linear vector space which may include states that are not normalizable according to the standard metrics. Indeed, it is just such an extension which seems to be necessitated by the CC parametrizations of the state vectors. One of the great attractions of the Bargmann representation is that it allows us to translate all such questions into specific problems in the theory of complex functions. In this way we can bring to bear some of the powerful results

of complex analysis, rather than trying to deal with the properties of general unnormalizable states in an abstract vector space.

In the first place we therefore consider the detailed mapping between the Schrödinger and holomorphic representations for *arbitrary* ket and bra wave functions $|\psi\rangle$ and $\langle\tilde{\psi}|$, parametrized respectively in the CIM form as

$$\begin{aligned} |\psi\rangle &= F(a^\dagger) |0\rangle; & \langle\tilde{\psi}| &= \langle 0| \tilde{F}(a), \\ F(z) &= \sum_{n=0}^{\infty} f_n z^n; & \tilde{F}(z) &= \sum_{n=0}^{\infty} \tilde{f}_n z^n. \end{aligned} \quad (3.22)$$

Their coordinate-space representations are the usual Schrödinger wave functions,

$$\langle x|\psi\rangle \equiv \psi(x); \quad \langle\tilde{\psi}|x\rangle \equiv \tilde{\psi}(x). \quad (3.23)$$

For the case of a Hermitian Hamiltonian as considered here, we have

$$\begin{aligned} \tilde{F}(z) &= N^{-2} F^*(z); & \langle\tilde{\psi}| &= N^{-2} (|\psi\rangle)^\dagger \\ N^2 &\equiv \langle\psi|\psi\rangle = \int_{-\infty}^{\infty} dx |\psi(x)|^2, \end{aligned} \quad (3.24)$$

with the normalization for $\langle\tilde{\psi}|$ as used in Section II, namely,

$$\begin{aligned} 1 &= \langle\tilde{\psi}|\psi\rangle = \int_{-\infty}^{\infty} dx \tilde{\psi}(x) \psi(x) \\ &= \langle 0| \tilde{F}(a) F(a^\dagger) |0\rangle = \sum_{n=0}^{\infty} n! \tilde{f}_n f_n. \end{aligned} \quad (3.25)$$

The intermediate normalization convention for $|\psi\rangle$ introduced in Section II,

$$1 = \langle 0|\psi\rangle = \int_{-\infty}^{\infty} dx \phi^*(x) \psi(x), \quad (3.26)$$

also implies the equivalent relation,

$$F(0) = f_0 = 1. \quad (3.27)$$

By making use of Eqs. (3.22), (3.15), and (A7), we find immediately that

$$\langle z^*|\psi\rangle = \langle z^*| F(a^\dagger) |0\rangle = F(z) \exp(-\tfrac{1}{2}|z|^2). \quad (3.28)$$

The insertion of a complete set of position eigenstates $|x\rangle$ into Eq. (3.28) and the use of Eq. (A11), then leads to the Fourier-like mapping,

$$F(z) = \pi^{-1/4} \exp(-\tfrac{1}{2}z^2) \int_{-\infty}^{\infty} dx \exp(\sqrt{2}zx - \tfrac{1}{2}x^2) \psi(x), \quad (3.29)$$

between the holomorphic and Schrödinger representations of an arbitrary wave function, $F(z)$ and $\psi(x)$, respectively. By considering the Fourier transform of Eq. (3.29), or by similarly considering the overlap $\langle x | \psi \rangle$ and inserting a complete set of coherent states as in Eq. (A8), one may also derive the inverse relations,

$$\psi(x) = 2^{-1/2} \pi^{-3/4} \exp(\tfrac{1}{2}x^2) \int_{-\infty}^{\infty} d\eta \exp(-i\sqrt{2}x\eta - \tfrac{1}{2}\eta^2) F(i\eta) \quad (3.30a)$$

$$= \pi^{-5/4} \exp(-\tfrac{1}{2}x^2) \int d^2z \exp(-|z|^2 - \tfrac{1}{2}z^{*2} + \sqrt{2}xz^*) F(z). \quad (3.30b)$$

Finally, we turn our attention to the specific case of the symmetric-well anharmonic oscillator (AO) systems for which the potential function is specified as

$$V(\xi) = 2^{-1-K} \lambda \xi^{2K}, \quad K = 2, 3, \dots, \quad (3.31)$$

and for which the ground-state solution is given in Schrödinger form from Eq. (3.1) by the solution to the differential equation

$$-\tfrac{1}{2}\psi_0''(x) + \tfrac{1}{2}\lambda x^{2K}\psi_0(x) = E_0\psi_0(x). \quad (3.32)$$

The physical ground-state solution $\psi_0(x)$ is clearly a symmetric, non-negative function. Its asymptotic behaviour is readily found from Eq. (3.32) in the standard fashion as

$$\psi_0(x) = \text{const} \times e^{Q(x)}$$

$$Q(x) \xrightarrow{x \rightarrow \pm\infty} -\frac{\sqrt{\lambda}}{(K+1)} |x|^{K+1} - \frac{1}{2} K \ln|x| + O(x^{1-K}). \quad (3.33)$$

Its holomorphic counterpart $F^0(z) \equiv \exp(-\tfrac{1}{2}z^2)f^0(z)$ may be found either from Eq. (3.29) or, directly, from Eq. (3.21) as the solution to the differential equation

$$\left(\frac{d}{dz}\right)^{2K} f^0(z) = \frac{2^{K+1}}{\lambda} \left[\left(\frac{1}{2} \frac{d}{dz} - z\right)^2 + E_0 \right] f^0(z). \quad (3.34)$$

Equation (3.29) and the knowledge that $\psi_0(x)$ is a real, positive function of even parity, immediately yield that $f^0(z)$ is an even entire function of z which is itself also real and positive on the real axis. The zeros of $f^0(z)$ must therefore lie outside a region surrounding the real axis. The further analytic properties of both functions $\psi_0(z)$ and $f^0(z)$ are examined in Appendix B.

It is clear by similar arguments to those used in Appendix B that *general* eigenstates $|\psi\rangle$ of the Hamiltonian in the AO Hilbert space have Schrödinger representations $\psi(x)$ which, since $V(\sqrt{2}x)$ is an analytic function of x , may be analytically continued into the complex plane where they are entire functions of order $(K+1)$. Their corresponding holomorphic representations $F(z) =$

$\exp(-\frac{1}{2}z^2)f(z)$ have entire functions $f(z)$ of fractional order $\nu = (K+1)/K$, with $1 < \nu < 2$. They may therefore be represented by the well-known Hadamard decomposition theorem in terms of a product over their infinite set of zeros z_m , such that $f(z_m) = 0$,

$$F(z) = z^n \exp\left(-\frac{1}{2}z^2 + f_1 z\right) \prod_m \left(1 - \frac{z}{z_m}\right) \exp\left(\frac{z}{z_m}\right), \quad (3.35)$$

where for even eigenstates $n=0$, where we have explicitly used the intermediate normalization of Eq. (3.27), and where we have also made explicit the dependence on the first odd coefficient f_1 . The remaining coefficients $\{f_n; n=2, 3, \dots\}$ are clearly wholly determined by the zeros $\{z_m\}$. For the special case of the stationary ground state $|\psi_0\rangle$, $F(z) \rightarrow F^0(z)$, which is an even function, so that $f_1^0 = 0$ and the zeros must therefore appear in symmetric pairs $z_m^0 \rightarrow \pm \zeta_m$. The distribution of the zeros of $F^0(z)$ is investigated in more detail in Appendix B.

In Section IV we next turn our attention to the analytic properties of the corresponding holomorphic representations of the respective operators $\{X, \tilde{X}\}$ that characterize the remaining two IC parametrizations, namely the NCCM and ECCM, for the one-mode bosonic field theories.

IV. THE COUPLED-CLUSTER AMPLITUDE FUNCTIONS

IV.1. The Operators $\tilde{S}$ and $\tilde{X}$

In the NCCM the operator $\tilde{S} = \tilde{S}(a)$ is given by Eq. (2.8), which for the time-independent case where $k=1$ is specified as

$$\langle 0 | \tilde{S}(a) = \frac{\langle 0 | \tilde{F}(a) F(a^\dagger)}{\langle 0 | \tilde{F}(a) F(a^\dagger) | 0 \rangle}, \quad (4.1)$$

in terms of the CIM operators. In the normalization scheme of Section III given by Eq. (3.25), we thus have from Eq. (3.17) the equivalent holomorphic representation

$$\tilde{S}(z) = F(d/dz) \tilde{F}(z). \quad (4.2)$$

If we write $\tilde{S}(z)$ in the same normalization scheme as in Section III as

$$\tilde{S}(z) = \sum_{n=0}^{\infty} \tilde{s}_n z^n; \quad \tilde{s}_0 = 1, \quad (4.3)$$

then it is immediately clear from Eq. (3.8) that the coefficients $\{\tilde{s}_n\}$ are given by

$$\tilde{s}_n = \frac{1}{n!} \langle 0 | \tilde{S} (a^\dagger)^n | 0 \rangle. \quad (4.4)$$

By recalling the NCCM parametrization of Eq. (2.8) and that $S = S(a^\dagger)$, Eq. (4.4) may be rewritten in the form

$$\begin{aligned}\tilde{s}_n &= \frac{1}{n!} \langle 0 | \tilde{S} e^{-S} (a^\dagger)^n e^S | 0 \rangle \\ &= \frac{1}{n!} \langle \tilde{\psi} | (a^\dagger)^n | \psi \rangle \equiv \frac{1}{n!} \langle (a^\dagger)^n \rangle,\end{aligned}\quad (4.5)$$

where, for an arbitrary operator $\mathcal{O} = \mathcal{O}(a^\dagger, a)$,

$$\bar{\mathcal{O}} \equiv \langle \mathcal{O} \rangle \equiv \langle \tilde{\psi} | \mathcal{O} | \psi \rangle. \quad (4.6)$$

Equations (4.3) and (4.5) yield the expression

$$\tilde{S}(z) = \langle \exp(za^\dagger) \rangle \equiv e^{\tilde{\Sigma}(z)}, \quad (4.7)$$

where in the last identity we have introduced the ECCM operator, $\tilde{\Sigma} = \tilde{\Sigma}(a)$ as in the general equation (2.10),

$$\tilde{\Sigma}(z) = \sum_{n=1}^{\infty} \tilde{\sigma}_n z^n. \quad (4.8)$$

It is clear from Eq. (4.7) that $\tilde{\Sigma}(z)$ is just the associated cumulant function whose coefficients $\tilde{\sigma}_n$ provide a measure of the *connected averages* of the powers of the creation operator $a^\dagger$,

$$\tilde{\sigma}_n = \frac{1}{n!} \langle (a^\dagger)^n \rangle_{\text{conn.}}. \quad (4.9)$$

Thus, the relationship between the (unlinked) coefficients $\{\tilde{s}_n\}$ and the (linked) coefficients $\{\tilde{\sigma}_n\}$ is just the usual one between the moments and cumulants of a probability distribution.

The function $\tilde{S}(z)$ may also be related to the Schrödinger wavefunction $\psi(x)$ by inserting a complete set of position eigenstates into the definition (4.7),

$$\tilde{S}(z) = \int_{-\infty}^{\infty} dx \langle \tilde{\psi} | x \rangle \langle x | e^{za^\dagger} | \psi \rangle. \quad (4.10)$$

We may then use Eq. (3.2) to write the exponential operator in Eq. (4.10) in the form $\exp(za^\dagger) = \exp[2^{-1/2}z(x - d/dx)]$. A straightforward use of the Baker–Campbell–Hausdorff theorem then readily yields the explicit representation,

$$\tilde{S}(z) = \exp(-\frac{1}{4}z^2) \int_{-\infty}^{\infty} dx \exp(xz/\sqrt{2}) \tilde{\psi}(x) \psi(x - z/\sqrt{2}). \quad (4.11)$$

We note that Eq. (4.11) agrees with the convention $\tilde{s}_0 = \tilde{S}(0) = 1$, by the chosen normalization scheme of Eq. (3.25).

For the particular example of the ground state $|\psi_0\rangle$ of the AO systems of order $2K$ discussed in Section III, the qualitative properties of the corresponding function $\tilde{S}^0(z)$ are readily established using the properties of $\psi_0(x)$ given above. A detailed derivation is given in Appendix C, from which we find in particular that: (i) $\tilde{S}^0(z)$ is analytic in the whole complex z -plane and is an entire function of order $K+1$; (ii) the asymptotic behaviour of $\tilde{S}^0(z)$ along the real axis is given by

$$\begin{aligned}\tilde{S}^0(x) &\propto \exp(-d\sqrt{\lambda}|x|^{K+1}), & x \rightarrow \pm\infty, \\ d &\equiv (K+1)^{-1}2^{-(3K+1)/2},\end{aligned}\tag{4.12}$$

and (iii) $\tilde{S}^0(z)$ has no zeros in a strip surrounding the real axis. This last property ensures in particular that the amplitudes $\{\tilde{\sigma}_n\}$ exist and are uniquely determined by the expansion of $\ln \tilde{S}(z)$ around $z=0$.

More generally, it is evident that the function $\tilde{S}(z)$ is only properly defined if the corresponding Schrödinger wave function $\psi(x)$ satisfies certain quite stringent requirements. Indeed, such considerations lead us to the general problem of the “coupled cluster representability” (or CC-representability) of states in a Hilbert space. Since by Eq. (3.29) the holomorphic wave function $F(z)$, together with $S(z)=\ln F(z)$, exists and is well defined for arbitrary $\psi(x)$, the crucial test is the existence of the analytic function $\tilde{S}(z)$.

In this latter regard, it is not difficult to construct examples for which $\tilde{S}(z)$ is problematic. By way of illustration, if $\psi(x)$ has cusps or discontinuities in higher-order derivatives, the moments $\langle (a^\dagger)^n \rangle$ of Eq. (4.5) will clearly not exist for n greater than some value n_0 . Nevertheless it is apparent that an arbitrary $\psi(x) \in L_2[-\infty, \infty]$ can be obtained as the limit of a Cauchy sequence of functions $\phi_\nu(x) \in C^\infty$, such that for each such ϕ_ν the corresponding function $\tilde{S}_\nu(z)$ exists and is an entire function in the whole complex plane. However, although the sequence ϕ_ν converges to ψ in $\mathcal{H}$, the sequence $\tilde{S}_\nu(z)$ does not necessarily converge to a limit in the space of all complex functions. On the other hand, the above argument still proves that the CC-representable states are dense in the Hilbert space $\mathcal{H} = L_2[-\infty, \infty]$. Henceforth we shall restrict our analysis to the class of CC-representable states and assume that the Hamiltonian is also regular enough so as to maintain the CC-representability during temporal evolution.

For further discussion we shall also need the Fourier transform $\tilde{S}_F(q)$ of $\tilde{S}(z)$ evaluated along the real axis, where

$$\tilde{S}(x) = \int_{-\infty}^{\infty} \frac{dq}{2\pi} e^{iqx} \tilde{S}_F(q), \quad x \in \mathbb{R},\tag{4.13a}$$

and with the corresponding inverse relation,

$$\tilde{S}_F(q) = \int_{-\infty}^{\infty} dx e^{-iqx} \tilde{S}(x).\tag{4.13b}$$

Equation (4.2) then immediately yields the relation

$$\tilde{S}_F(q) = F(iq) \tilde{F}_F(q), \quad (4.14)$$

where $\tilde{F}_F(q)$ is the Fourier transform of $\tilde{F}(x)$ defined analogously to Eq. (4.13b). An alternative form, which can be either calculated directly from Eq. (4.11), or derived from Eq. (4.14) using the analogous relation to Eq. (3.30a) for $\tilde{\psi}(x)$ in terms of $\tilde{F}(z)$, is

$$\tilde{S}_F(q) = f(iq) \tilde{\chi}(q), \quad (4.15)$$

where $f(z)$ is given in terms of Eq. (3.29) as

$$f(z) \equiv e^{z^2/2} F(z), \quad (4.16)$$

and the function $\tilde{\chi}(q)$ is defined analogously as

$$\tilde{\chi}(q) \equiv 2^{1/2} \pi^{1/4} \int_{-\infty}^{\infty} dx \exp(\tfrac{1}{2}x^2 - i\sqrt{2}qx) \tilde{\psi}(x). \quad (4.17)$$

In more general cases than the anharmonic oscillator potentials considered here, one may need to consider some alternative directions in the complex z -plane, other than the real x -axis, along which $\tilde{S}(z)$ decreases asymptotically fast enough to allow the Fourier transform to be determined. A simple example is the harmonic oscillator of larger width than that of Eq. (3.5) which provides us with the model state $\phi(x)$. In this case $H \rightarrow H^0(\lambda) = \frac{1}{2}\hat{p}^2 + \frac{1}{2}\lambda\hat{x}^2$, with $\lambda < 1$, and $\psi_0(x)$ and $\tilde{\psi}_0(x)$ are proportional to $\exp(-\frac{1}{2}\sqrt{\lambda}x^2)$, so that the integral in Eq. (4.17) clearly diverges, for example, although $\tilde{S}(z)$ exists.

IV.2. The Operators S and Σ

As we have seen, the standard coupled-cluster amplitudes of the NCCM approach are defined as the cumulants of the holomorphic wave function,

$$S(z) \equiv \ln F(z) = \sum_{n=1}^{\infty} s_n z^n, \quad (4.18)$$

in the normalization of Eq. (3.27) with $f_0 = 1$. From the Hadamard decomposition of Eq. (3.35) for $F(z)$, we have

$$S(z) = f_1 z - \frac{1}{2} z^2 + \sum_m [\ln(1 - z/z_m) + z/z_m]. \quad (4.19)$$

We observe that $s_1 = f_1$ is formally independent of the zeros $\{z_m\}$ of $F(z)$, whereas the higher-order coefficients are given explicitly in terms of them as

$$s_n = -\frac{1}{2} \delta_{n,2} - \frac{1}{n} \sum_m z_m^{-n}; \quad n \geq 2. \quad (4.20)$$

For the class of AO states considered here the above sums are readily seen to converge, using the results of Appendix B. If $\rho = \min\{|z_m|\}$ is the distance of the nearest zero to the origin, the asymptotic behaviour of the NCCM amplitudes is given explicitly as

$$|s_n| \propto \frac{1}{n} \rho^{-n}; \quad n \rightarrow \infty. \quad (4.21)$$

It is also immediately clear that the state $S(a^\dagger)|0\rangle$ is not normalizable within $\mathcal{H}$ for the AO states. One obvious consequence is that the CCM operator $S(a^\dagger) = S$ cannot simply be reckoned to be an operator which generates "small" correlations in some suitably defined perturbative sense, even when one might otherwise naively intuit that this is the case, such as for small coupling constants, λ .

Let us now assume that a straight line L passing through the origin in the complex z -plane can be found such that it avoids all of the zeros $\{z_m\}$ of $F(z)$. Let L be in the direction of a unit vector $\eta = \exp(i\phi)$, where $-\frac{1}{2}\pi < \phi < \frac{1}{2}\pi$. Therefore there exists a strip surrounding L in which all of the singularities of $S(z)$ can be avoided by excluding all of the branch cuts. We may then use L to define the Fourier transform of the unique function $S(z)$ on L . We note that since $S(z)$ increases asymptotically as z^2 from Eq. (4.19), its Fourier transform (as well as $S(z)$ itself) is actually a generalized function or distribution, in the usual Schwartz sense [46]. In this regard we also note that for the symmetric AO case considered here $f_1 = 0$, and, from Appendix B, the sum over zeros in Eq. (4.19) behaves asymptotically as z^ν with $\nu = (K+1)/K$ for large values of z . Since $S(0) = 0$, it is convenient first to define a function $g(x)$ such that, for $z \in L$,

$$\begin{aligned} S(z) &= \int_{-\infty}^{\infty} dx (e^{i\eta^* z x} - 1) g(x) \\ &= g_F(-\eta^* z) - g_F(0), \end{aligned} \quad (4.22)$$

where $g_F(q)$ is the corresponding Fourier transform of $g(x)$, defined analogously to Eq. (4.13b).

A careful but essentially straightforward analysis based on Eqs. (4.19) and (4.22), then reveals that $g(x)$ may be written in the form

$$g(x) = i\eta f_1 \delta'(x) + \frac{1}{2} \eta^2 \delta''(x) + g^+(x) + g^-(x), \quad (4.23)$$

where the distributions $g^\pm(x)$ are given, for $x \in \mathbb{R}$, by

$$g^\pm(x) = \sum_m^{(\pm)} \left[\pm \frac{1}{x} \theta(\mp x) \exp(-i\eta^* z_m x) + \frac{i\eta}{z_m} \delta'(x) \right], \quad (4.24)$$

in terms of the usual step function $\theta(x) = \frac{1}{2}[1 + \text{sgn}(x)]$, with derivative $\theta'(x) = \delta(x)$, the Dirac delta. The sums denoted by $\sum_m^{(\pm)}$ in Eq. (4.24) have the following meaning. The zeros $\{z_m\}$ of $F(z)$ are first grouped into two classes according

to whether they lie to the left (+) or to the right (−) of the line L . Thus the sums $\sum_m^{(\pm)}$ in the expressions for $g^\pm(x)$ run over all zeros in the two half-planes, $z_m \in D_L^\pm$, respectively, where $D_L^\pm = \{z | \text{Im}(\pm z/\eta) > 0\}$. We emphasize again that the sums in Eq. (4.24) for $g^\pm(x)$ converge in the sense of generalized functions. Indeed they are defined in such a way as to minimize the degree of non-analyticity for $g^\pm(x)$ at $x=0$. The function $g(x)$ as given above is thus a regularized generalized function [46].

For the states of the symmetric AO (of order $2K$), the discussion in Appendix B on the distribution of the zeros of $F(z)$ for these cases, shows that we can let the direction η of the line L approach the imaginary axis ($\phi \rightarrow \frac{1}{2}\pi - \varepsilon$, where ε is a positive infinitesimal), so that $\eta \rightarrow i$ and

$$\begin{aligned} S(z) &= \int_{-\infty}^{\infty} dx (e^{xz} - 1) g(x) \\ &= g_F(iz) - g_F(0). \end{aligned} \quad (4.25)$$

Furthermore, we can readily show that the behaviour of $g(x)$ for small (but non-zero) values of x for the AO case is as

$$g(x) \propto |x|^{-\nu-1}; \quad |x| \rightarrow 0, \quad (4.26)$$

where $\nu = (K+1)/K$ as before. Finally, we remark that it is obvious that whereas $S(z)$ is a unique function, its representation in terms of $g(x)$ can be chosen in a variety of ways. A slightly different choice was made in Ref. [37], for example.

We turn now to the ECCM amplitudes $\{\sigma_n\}$ which play a comparable role to the amplitudes $\{s_n\}$ in the NCCM parametrization scheme. Following the general discussion of Section II, and paying attention to the normalization scheme introduced in Section III, we define the amplitudes $\{\sigma_n\}$ as in Eq. (2.12) by

$$\sigma_n = \frac{1}{n!} \langle 0 | \tilde{S}(a) a^n S(a^\dagger) | 0 \rangle; \quad n \geq 1. \quad (4.27)$$

The corresponding function $\Sigma(z)$ is given as,

$$\begin{aligned} \Sigma(z) &= \sum_{n=1}^{\infty} \sigma_n z^n \\ &= \langle 0 | \tilde{S}(a)(e^{za} - 1) S(a^\dagger) | 0 \rangle. \end{aligned} \quad (4.28)$$

By inserting the expansions (4.3) and (4.18) into Eq. (4.27) and using Eq. (3.8), we may readily derive the formal expansion

$$\sigma_n = \sum_{m=0}^{\infty} \frac{(m+n)!}{n!} \tilde{s}_m s_{m+n}. \quad (4.29)$$

A crucial problem in the definition of these ECCM amplitudes derives from the

fact that usually neither the state $S(a^\dagger)|0\rangle$ nor $\langle 0|\tilde{S}(a)$ is normalizable within $\mathcal{H}$. As already discussed, this lack of normalizability is intimately connected with the properties of the corresponding complex-valued functions $S(z)$ and $\tilde{S}(z)$ of the complex variable z . For example, it is rather readily proven (and see Appendix D) that for the states of the AO of order $2K$, the expansion (4.29) formally diverges. We remark in passing that such problems of convergence never occur in finite-dimensional Hilbert spaces.

In order to associate a well-defined meaning to the new ECCM amplitudes in the present case of an infinite Hilbert space, it is necessary to introduce a method of regularization for the formally divergent sum in Eq. (4.29). The approach we adopt is to work within the Bargmann representation. More specifically, we aim to demonstrate that a consistent interpretation can be given to such expressions as (4.27), and furthermore that the particular interpretation can be used everywhere within the whole IC formalism. In so doing it will become apparent that the chosen regularization scheme is not unique. This implies therefore that the nonlinear classical mapping of the original quantum problem afforded by the ECCM parametrization is not necessarily unique, but is rather one-to-many. Nevertheless, we emphasize at this early stage that even though the values of the individual amplitudes $\{\sigma_n; n=2, 3, \dots\}$ may in principle be chosen in a variety of ways, the expressions for the average values of operators remain unique. The additional degrees of freedom in the present case are very reminiscent of the gauge degrees of freedom in gauge field theories, and a particular choice for them corresponds to gauge fixing. A more careful analysis of these questions will be postponed to the sequel of the present paper (II).

We proceed as follows. Equation (4.28) formally gives us the result

$$\begin{aligned}\Sigma(z) &= \tilde{S}(d/du)[\exp(zd/du) - 1] S(u)|_{u=0} \\ &= \tilde{S}(d/du)[S(u+z) - S(u)]|_{u=0}.\end{aligned}\quad (4.30)$$

The coefficients are similarly obtained from Eq. (4.27) in the form

$$\sigma_n = \frac{1}{n!} \tilde{S}(d/du) S^{(n)}(u)|_{u=0}; \quad n \geq 1, \quad (4.31)$$

where $f^{(n)}(x) \equiv d^n f/dx^n$. In keeping with the earlier discussion we consider again the straight line L through the origin in the z -plane on which $S(z)$ may be defined as a unique analytic function, and apply the representation of Eq. (4.22) to Eq. (4.31). We thereby obtain the result,

$$\sigma_n = \frac{(i\eta^*)^n}{n!} \int_{-\infty}^{\infty} dx x^n \tilde{S}(i\eta^* x) g(x), \quad n \geq 1, \quad (4.32)$$

and hence, from Eq. (4.28),

$$\Sigma(z) = \int_{-\infty}^{\infty} dx (e^{i\eta^* z x} - 1) \tilde{S}(i\eta^* x) g(x). \quad (4.33)$$

Once again we can let $\eta \rightarrow i$ for the AO class of states, to obtain in that case,

$$\Sigma(z) = \int_{-\infty}^{\infty} dx (e^{xz} - 1) \gamma(x), \quad (4.34)$$

where the function $\gamma(x)$ is defined for $x \in \mathbb{R}$ as

$$\gamma(x) \equiv \tilde{S}(x) g(x). \quad (4.35)$$

Equation (4.34) for the ECCM function $\Sigma(z)$ is the obvious counterpart of Eq. (4.25) for its NCCM analogue $S(z)$. We note that the strongly vanishing asymptotic behaviour of $\tilde{S}(x)$ for $|x| \rightarrow \infty$, given by Eq. (4.12), ensures that Eq. (4.34) defines $\Sigma(z)$ directly for all values of z as an entire function. This in turn implies that the coefficients $\{\sigma_n\}$ decrease for large n more rapidly than any power. By contrast, the asymptotic behaviour of $g(x)$ for $|x| \rightarrow \infty$ ensures that Eq. (4.25) only similarly defines $S(z)$ on the line L , whence it can be analytically continued, however.

The spirit of the regularization method introduced above is based on the identification of the coupled-cluster degrees of freedom with the values of $S(z)$ on the fixed line $z \in L$ around which $S(z)$ is analytic and unique. This set of values is complete in the sense that they suffice to define $S(z)$ everywhere by analytic continuation. Thus they also define the holomorphic wave function $F(z) = \exp[S(z)]$, and thereby the original quantum-mechanical state in the Hilbert space $\mathcal{H}$. The amplitudes $\{\sigma_n\}$, however, must at this level be considered somewhat artificial constructs, for which no obvious interpretation can be given in terms of the properties of $\mathcal{H}$. Instead, they are very intimately connected with the linked diagram expansions. We explain in some detail in the subsequent paper (II) their interpretation in terms of the important ECCM tree diagrams.

IV.3. The Temporal Action

It is instructive to evaluate the temporal part $\mathcal{A}_0$ of the action functional of Eq. (2.4),

$$\mathcal{A}_0 = \int_{t_1}^{t_2} dt \langle \tilde{\Psi}(t) | i\partial/\partial t | \psi(t) \rangle, \quad (4.36)$$

for each of the IC parametrizations. We note in passing that, due to the intermediate normalization condition employed for the CC parametrizations, the temporal action $\mathcal{A}_0$ in the CC cases turns out to be precisely the Berry phase in those particular applications involving adiabatic changes.

In the case of the CIM it is usual not to normalize the bra and ket states explicitly. Instead, the normalization may be included as an additional constraint later, since the overlap $\langle \tilde{\Psi} | \psi \rangle$ is conserved under time evolution. We have immediately from Eqs. (3.11) and (3.22)

$$\mathcal{A}_0^{\text{CIM}} = i \int_{t_1}^{t_2} dt \tilde{F}(d/dz) \dot{F}(z)|_{z=0}, \quad (4.37)$$

where $\dot{f} \equiv df/dt$ as usual, and the explicit time dependence of the various holomorphic functions is here and henceforth suppressed. For the AO class of functions, $F(z)$ asymptotically strongly decreases along the real axis, and we therefore represent it analogously to Eq. (4.13a) by the Fourier transform $F_F(q) \equiv 2\pi\Phi(q)$,

$$F(z) = \int_{-\infty}^{\infty} dx e^{ixz} \Phi(x); \quad z \in \mathbb{R}. \quad (4.38)$$

By insertion of Eq. (4.38) into Eq. (4.37), we find

$$\mathcal{A}_0^{\text{CIM}} = i \int_{t_1}^{t_2} dt \int_{-\infty}^{\infty} dx \tilde{\Phi}(x) \dot{\Phi}(x), \quad (4.39)$$

where

$$\tilde{\Phi}(x) \equiv \tilde{F}(ix). \quad (4.40)$$

The discussion of Sections II and III shows that the analogue of Eq. (4.37) for the NCCM is

$$\begin{aligned} \mathcal{A}_0^{\text{NCCM}} &= \int_{t_1}^{t_2} dt \langle 0 | \tilde{S} e^{-S(i\partial/\partial t)} e^S | 0 \rangle \\ &= i \int_{t_1}^{t_2} dt \tilde{S}(d/dz) \dot{S}(z)|_{z=0}. \end{aligned} \quad (4.41)$$

By inserting the representation of Eq. (4.25) for $S(x)$, we find

$$\mathcal{A}_0^{\text{NCCM}} = i \int_{t_1}^{t_2} dt \int_{-\infty}^{\infty} dx [\tilde{S}(x) - \tilde{S}(0)] \dot{g}(x). \quad (4.42)$$

By using the explicit normalization within the NCCM that $\tilde{S}(0) = s_0 = 1$, independent of time, we can neglect the second term in Eq. (4.42) as usual as being a total time derivative, to arrive at the final result,

$$\mathcal{A}_0^{\text{NCCM}} = i \int_{t_1}^{t_2} dt \int_{-\infty}^{\infty} dx \tilde{S}(x) \dot{g}(x). \quad (4.43)$$

Finally, the analogous ECCM representation of $\mathcal{A}_0$ may be written using Eq. (4.7). By using the definition (4.35) and by adding the (irrelevant) total time derivative, $(d/dt)(\gamma\tilde{S} - g\tilde{S})$, to the integrand in Eq. (4.43), we obtain the final form,

$$\mathcal{A}_0^{\text{ECCM}} = i \int_{t_1}^{t_2} dt \int_{-\infty}^{\infty} dx \tilde{S}(x) \dot{\gamma}(x). \quad (4.44)$$

A comparison of the three corresponding IC parametrizations of $\mathcal{A}_0$ of Eqs. (4.39), (4.43), and (4.44) shows how their generic form may be given in terms of a bilinear

product of $\tilde{X}(z)$ and a suitable Fourier transform of $X(z)$, where $\{X, \tilde{X}\}$ are the canonically conjugate generic IC operators. Expressed equivalently using their n -body expansion coefficients $\{x_n, \tilde{x}_n\}$, it is trivial to derive the corresponding results,

$$\mathcal{A}_0^{\text{CIM}} = i \int_{t_1}^{t_2} dt \sum_{n=0}^{\infty} n! \tilde{f}_n \dot{f}_n, \quad (4.45a)$$

$$\mathcal{A}_0^{\text{NCCM}} = i \int_{t_1}^{t_2} dt \sum_{n=1}^{\infty} n! \tilde{s}_n \dot{s}_n, \quad (4.45b)$$

$$\mathcal{A}_0^{\text{ECCM}} = i \int_{t_1}^{t_2} dt \sum_{n=1}^{\infty} n! \tilde{\sigma}_n \dot{\sigma}_n. \quad (4.45c)$$

The appearance of the factors $n!$ in Eqs. (4.45a)–(4.45c) is directly related to the normalization scheme adopted for the one-mode bosonic field theories, in comparison with the general convention adopted in Section II.

V. IC GENERATING FUNCTIONALS FOR EXPECTATION VALUES

In each of the three IC methods both the bra and ket vectors are given and parametrized in terms of the corresponding sets of canonical variables. We may therefore form a density matrix which allows the calculation of all physical properties of the system in terms of the expectation values of appropriate operators. A very convenient way to obtain such expectation values is to introduce a suitable generating functional for them. For this purpose we introduce the expectation value $A(u, v)$ of the following biexponential operator,

$$A(u, v) \equiv \langle \tilde{\psi} | e^{ua^\dagger} e^{va} | \psi \rangle \equiv \langle e^{ua^\dagger} e^{va} \rangle, \quad (5.1)$$

for normalized states, $\langle \tilde{\psi} | \psi \rangle = 1$. If an arbitrary operator $\mathcal{O} = \mathcal{O}(a^\dagger, a)$ is now specified in normal-ordered form (with respect to the operators a and $a^\dagger$), $\mathcal{O} \equiv : \mathcal{O} :$, its expectation value, $\bar{\mathcal{O}} \equiv \langle \tilde{\psi} | \mathcal{O} | \psi \rangle \equiv \langle \mathcal{O} \rangle$, can be calculated as

$$\bar{\mathcal{O}} = \mathcal{O}(\partial_u, \partial_v) A(u, v)|_{u=v=0}, \quad (5.2)$$

where $\partial_u = \partial/\partial u$, $\partial_v = \partial/\partial v$.

It is also straightforward to calculate the expectation values of operators that depend only on the position or momentum operators, $\hat{x}$ and $\hat{p}$, respectively. Thus, one may use the Baker–Campbell–Hausdorff theorem to write

$$\begin{aligned} \langle \exp(\sqrt{2} u \hat{x}) \rangle &= \langle \exp u(a^\dagger + a) \rangle \\ &= e^{u^2/2} \langle e^{ua^\dagger} e^{ua} \rangle, \end{aligned} \quad (5.3)$$

and hence

$$\langle \phi(\sqrt{2} \hat{x}) \rangle = \phi(\partial_u) e^{u^2/2} A(u, u)|_{u=0}. \quad (5.4)$$

Similarly, we also find the result,

$$\langle \phi(\sqrt{2} \hat{p}) \rangle = \phi(\partial_u) e^{u^2/2} A(iu, -iu)|_{u=0}. \quad (5.5)$$

As a specific example, the kinetic energy has an expectation value given by

$$\langle \frac{1}{2} \hat{p}^2 \rangle = \frac{1}{4} [1 - (\partial_u - \partial_v)^2] A(u, v)|_{u=v=0}. \quad (5.6)$$

We now proceed to formulate the generating functional for each of the three IC parametrizations. For the CIM we first use the result of Eq. (3.13) to write $A(u, v)$ in terms of a double integral over the complex plane. This is most readily done by first interchanging the order of the exponential factors by using the simple relation

$$e^{ua^\dagger} e^{va} = e^{-uv} e^{va} e^{ua^\dagger}. \quad (5.7)$$

Equation (3.13) then readily yields the result,

$$A(u, v) = \frac{1}{\pi} \int d^2 z e^{-|z|^2 - uv} \tilde{F}(z^*) e^{vz^*} e^{uz} F(z). \quad (5.8)$$

A simple shift of origin so that $z \rightarrow z + v$, $z^* \rightarrow z^* + u$, then allows us to rewrite Eq. (5.8) in the form

$$A(u, v) = \frac{1}{\pi} \int d^2 z e^{-|z|^2} \tilde{F}(z^* + u) F(z + v). \quad (5.9)$$

The alternative choice of Eq. (3.11) for the scalar product, which is based on the Bargmann algebra (3.14), first gives the expression

$$A(u, v) = \tilde{F}(d/dz) e^{uz} e^{vd/dz} F(z)|_{z=0} \quad (5.10)$$

as another way of writing the CIM generating functional. By making use of the elementary operator relations

$$\frac{d}{dz} e^{uz} = e^{uz} \left(\frac{d}{dz} + u \right); \quad e^{vd/dz} z = (z + v) e^{vd/dz}, \quad (5.11)$$

we may rewrite Eq. (5.10) in the form

$$A(u, v) = \tilde{F}(u + d/dz) F(v + z)|_{z=0}. \quad (5.12)$$

If the function F is then represented through its Fourier transform F_F , defined as in Eq. (4.13a) we may also express Eq. (5.12) in the CIM form

$$\begin{aligned} A(u, v) &= \int_{-\infty}^{\infty} \frac{dq}{2\pi} \tilde{F}(u + iq) e^{iqv} F_F(q) \\ &= \int_{-\infty}^{\infty} dx \tilde{\Phi}(x - iu) e^{ixv} \Phi(x), \end{aligned} \quad (5.13)$$

where in the second equality we have used the definitions in Eqs. (4.38)–(4.40). Alternatively, if the function $\tilde{F}$ in Eq. (5.12) is represented by its Fourier transform $\tilde{F}_F$, defined again as in Eq. (4.13a), Eq. (5.12) can also be written in the CIM form

$$A(u, v) = \int_{-\infty}^{\infty} \frac{dq}{2\pi} \tilde{F}_F(q) e^{iqu} F(v + iq). \quad (5.14)$$

Equations (5.13) and (5.14) lead quite trivially to the explicit expressions,

$$\langle (a^\dagger)^n a^m \rangle = i^m \int_{-\infty}^{\infty} \frac{dq}{2\pi} q^m \tilde{F}^{(n)}(iq) F_F(q) \quad (5.15a)$$

$$= i^n \int_{-\infty}^{\infty} \frac{dq}{2\pi} q^n \tilde{F}_F(q) F^{(m)}(iq). \quad (5.15b)$$

Either by expanding Eqs. (5.15a), (5.15b), or by direct use of Eq. (5.12), it is easy to show also that this latter expectation value can be written explicitly in terms of the CIM canonically conjugate set of coordinates $\{f_n, \tilde{f}_n\}$ as

$$\langle (a^\dagger)^n a^m \rangle = \sum_{l=0}^{\infty} \frac{(m+l)! (n+l)!}{l!} f_{m+l} \tilde{f}_{n+l}. \quad (5.15c)$$

For both of the CC parametrizations we start from the formal expression

$$\begin{aligned} A(u, v) &= \langle 0 | \tilde{S}(a) e^{-S(a^\dagger)} e^{ua^\dagger} e^{va} e^{S(a^\dagger)} | 0 \rangle \\ &= \tilde{S}(d/dz) e^{-S(z)} e^{uz} e^{vd/dz} e^{S(z)} \big|_{z=0}. \end{aligned} \quad (5.16)$$

By making use of Eq. (5.11), we may readily rewrite Eq. (5.16) in the simplified form

$$A(u, v) = \tilde{S}(u + d/dz) e^{S(z+v) - S(z)} \big|_{z=0}. \quad (5.17)$$

It follows from Eq. (4.25) that the exponent in Eq. (5.17) may be written as

$$S(z+v) - S(z) = \int_{-\infty}^{\infty} dx e^{xz} (e^{xv} - 1) g(x). \quad (5.18)$$

By expanding the exponential in Eq. (5.17) as a power series, we obtain the NCCM result,

$$A(u, v) = \sum_{n=0}^{\infty} \frac{1}{n!} \prod_{i=1}^n \left[\int_{-\infty}^{\infty} dx_i (e^{x_i v} - 1) g(x_i) \right] \tilde{S}(u + x_1 + \cdots + x_n). \quad (5.19)$$

Before proceeding to the corresponding result for the ECCM it is worth considering the structure of Eq. (5.19) in more detail. As we already know, in the NCCM the canonically conjugate basic variables are the coordinates $\{s_n, \tilde{s}_n\}$, as is clearly shown by the form (4.45b) for the temporal action, for example. In the continuous (holomorphic) representation of Eq. (4.43), the canonically conjugate pair of functions is $\{g(x), \tilde{S}(x)\}$. Nevertheless, this is completely equivalent to the previous case, since if $\tilde{S}(x)$ is expanded as the power series (4.3) with respect to x , and with coefficients $\{\tilde{s}_n\}$, one immediately obtains as second factors the moments of the generalized function $g(x)$. These latter are precisely the coefficients $\{s_n\}$, as may be seen from the defining relation (4.25),

$$s_n = \frac{1}{n!} \int_{-\infty}^{\infty} dx x^n g(x); \quad n \geq 1. \quad (5.20)$$

It is clear that in the NCCM generating functional of Eq. (5.19), the same canonically conjugate pair of functions $\{g(x), \tilde{S}(x)\}$ appears as in the temporal action, in complete analogy with their CIM counterparts (cf., Eqs. (4.39) and (5.13)) with respect to the canonically conjugate pair of functions $\{\Phi(x), \tilde{\Phi}(x)\}$ in that case.

If the function $\tilde{S}$ in Eq. (5.19) were to be expanded into a power series of its argument, with coefficients $\{\tilde{s}_n\}$, and the remaining exponential factors were similarly expanded, one would again obtain moments of the function g as above. In this manner the functional $A(u, v)$ would become expressed entirely in terms of the canonical NCCM variables $\{s_n, \tilde{s}_n\}$ as the analogue of the corresponding CIM functional of Eq. (5.15c), for example. Nevertheless, such an expression for the NCCM case, when given explicitly in terms of the n -body cluster amplitudes $\{s_n, \tilde{s}_n\}$, is certainly much more complicated than the compact functional representation of Eq. (5.19) in terms of the functions $\{g(x), \tilde{S}(x)\}$. One of the main aims of the subsequent paper (II) is to give a more complete discussion of these aspects and their diagrammatic interpretation. We remark also that in order to emphasize the functional structure of the average-value generator A , we should write it in one of the complete forms,

$$\begin{aligned} A &= A[u, v; g(x), \tilde{S}(x)] \\ &= A[u, v; \{s_n, \tilde{s}_n\}], \end{aligned} \quad (5.21)$$

in the NCCM parametrization, for example, and similarly for the other IC schemes. We also note that in the case of an operator $\mathcal{O}(a^\dagger, a)$ which is a finite-order polynomial in $a^\dagger$ and a , its corresponding NCCM average value obtained from Eq. (5.19) is also a finite-order multinomial of the variables $\{s_n, \tilde{s}_n\}$.

We turn finally to the ECCM case wherein the functional A is formulated in terms of the canonical functions $\{\gamma(x), \tilde{\Sigma}(x)\}$, where $\gamma(x)$ is defined in Eq. (4.35). The necessary replacement is most easily performed on the final NCCM expression (5.19). From the basic definitions of Eqs. (4.7) and (4.35) we immediately obtain,

$$\begin{aligned} A &= A[u, v; \gamma(x), \tilde{\Sigma}(x)] \\ &= \sum_{n=0}^{\infty} \frac{1}{n!} \prod_{i=1}^n \left[\int_{-\infty}^{\infty} dx_i (e^{x_i v} - 1) \gamma(x_i) \right] \\ &\quad \times \exp[\tilde{\Sigma}(u + x_1 + \cdots + x_n) - \tilde{\Sigma}(x_1) - \cdots - \tilde{\Sigma}(x_n)]. \end{aligned} \quad (5.22)$$

Once again, the sum over n in Eq. (5.22) truncates after a finite number of terms in the case of evaluating the average value for an operator $\mathcal{O}$ of finite order in $a^\dagger$ and a . The ECCM generating functional may also be expressed in the form $A = A[u, v; \{\sigma_n, \tilde{\sigma}_n\}]$ by expanding the various functions $\tilde{\Sigma}$ in the exponent in Eq. (5.22) and by using the property that the amplitudes $\{\sigma_n\}$ are given by the moments of the generalized function $\gamma(x)$,

$$\sigma_n = \frac{1}{n!} \int_{-\infty}^{\infty} dx x^n \gamma(x); \quad n \geq 1, \quad (5.23)$$

by using Eq. (4.34).

By contrast with the NCCM case, the ECCM expansions in terms of $\{\sigma_n, \tilde{\sigma}_n\}$ are much more complicated than those in terms of $\{s_n, \tilde{s}_n\}$. Thus, the average value for even a finite-order operator $\mathcal{O}$ in $a^\dagger$ and a is now an infinite-order multinomial of the coefficients $\{\tilde{\sigma}_n\}$, although still of finite order with respect to the coefficients $\{\sigma_n\}$. It is clear that all such infinite-order expansions in the CC cases may have inherent convergence problems related to the arbitrariness or multitude of ways in which the terms in the discrete sums are arranged. By contrast, we emphasize that the functional expressions (5.19) and (5.22), for the NCCM and ECCM parametrizations in terms of the conjugate pairs of functions $\{g(x), \tilde{S}(x)\}$ and $\{\gamma(x), \tilde{\Sigma}(x)\}$, respectively, are rigorously convergent and well defined for arbitrary values of u and v for the AO systems.

A particularly compact form of the NCCM generating functional of Eq. (5.19) may be given by writing the function $\tilde{S}$ in terms of its Fourier transform $\tilde{S}_F$ from Eq. (4.13a). By making further use of Eq. (4.25) we readily derive the expression

$$\begin{aligned} A(u, v) &= \int_{-\infty}^{\infty} \frac{dq}{2\pi} \tilde{S}_F(q) e^{iqu + B(v, q)}, \\ B(v, q) &\equiv S(v + iq) - S(iq), \end{aligned} \quad (5.24)$$

which may be compared with its CIM counterpart of Eq. (5.14). Indeed this latter result (5.24) may be directly obtained from the earlier result (5.14) by using Eqs. (4.14) and (4.18). It could also have been derived rather easily from Eq. (5.17).

The argument iq in the function $S(iq)$ of Eq. (5.24) needs to be handled with caution in order to avoid the branch points $\{z_m\}$ of $S(z)$ on the imaginary axis. From our preceding discussion it is clear that iq should be understood as the limit of ηq as the argument ϕ of the unit vector $\eta = \exp(i\phi)$ approaches $\frac{1}{2}\pi$ from below. However, we also observe that whereas $B(v, q)$ is not single-valued in view of the logarithmic branch points, the corresponding function $\exp[B(v, q)] = F(v + iq)/F(iq)$ is single-valued. Furthermore, the poles in $\exp(B)$ at the zeros of $F(iq)$ are cancelled in the integrand of Eq. (5.24) by the corresponding zeros in $\tilde{S}_F(q)$ at the same points, from Eq. (4.14). For the case of the AO systems, Eq. (4.19) shows that the asymptotic behaviour of $B(v, q)$ at $q \rightarrow \pm\infty$ is $B(v, q) \rightarrow -iqv$. Thus, the expression (5.24) for $A(u, v)$ is clearly well defined and convergent for real values of u and v . By analytic continuation it can then readily be proven to be analytic in the whole complex u and v planes.

We conclude this section by formulating the complete action functional of Eq. (2.4) for each of the three IC methods. It is convenient to rewrite the Hamiltonian of Eq. (3.1) for this purpose, by putting $V(z) \equiv \frac{1}{4}z^2 + U(z)$,

$$\begin{aligned} H &= \frac{1}{2}\hat{p}^2 + \frac{1}{2}\hat{x}^2 + U(\sqrt{2}\hat{x}) \equiv H^0 + U \\ &= a^\dagger a + \frac{1}{2} + U(a^\dagger + a). \end{aligned} \quad (5.25)$$

From Eq. (5.2) we may express the expectation value of the harmonic oscillator energy as

$$\bar{H}^0 = (\partial_u \partial_v + \frac{1}{2}) A(u, v)|_{u=v=0}. \quad (5.26)$$

We now consider the evaluation of $\bar{U}$ in each of the three IC parametrizations in turn.

(i) CIM. A straightforward use of Eqs. (5.4) and (5.13) gives for the expectation value of the potential U ,

$$\begin{aligned} \bar{U} &= \int_{-\infty}^{\infty} \frac{dq}{2\pi} F_F(q) U(\partial_u) e^{u^2/2 + iqu} \tilde{F}(u + iq)|_{u=0} \\ &= \int_{-\infty}^{\infty} dx \Phi(x) U(ix + u + \partial_u) \tilde{\Phi}(x - iu)|_{u=0} \\ &= \int_{-\infty}^{\infty} dx \tilde{\Phi}(x) U(ix + i\partial_x) \Phi(x). \end{aligned} \quad (5.27)$$

The harmonic energy is similarly seen to be given as

$$\bar{H}^0 = \int_{-\infty}^{\infty} dx [\tilde{\Phi}'(x) x + \frac{1}{2}\tilde{\Phi}(x)] \Phi(x), \quad (5.28)$$

where, in the case where the states are explicitly normalized, $\langle 0 | \tilde{F} F | 0 \rangle = 1$, the last term is precisely $\frac{1}{2}$, since the normalization then implies the relation

$$\int_{-\infty}^{\infty} dx \tilde{\Phi}(x) \Phi(x) = 1. \quad (5.29)$$

The total action is thus specified in the CIM parametrization as

$$\mathcal{A} = \int_{t_1}^{t_2} dt \left\{ i \int_{-\infty}^{\infty} dx \tilde{\Phi}(x) \dot{\Phi}(x) - H[\Phi, \tilde{\Phi}] \right\}, \quad (5.30)$$

where $\bar{H} = \bar{H}^0 + \bar{U}$ is given by Eqs. (5.27) and (5.28).

(ii) NCCM. A straightforward derivation based on Eqs. (5.19) and (5.24) now gives

$$\bar{H} = \frac{1}{2} \tilde{S}(0) + \int_{-\infty}^{\infty} dx \tilde{S}'(x) x g(x) + \int_{-\infty}^{\infty} \frac{dq}{2\pi} \tilde{S}_F(q) U(iq + u + \partial_u) e^{B(u,q)}|_{u=0}. \quad (5.31)$$

When inserted into the action functional, the last term in Eq. (5.31), which gives the average-value functional $\bar{U}$, is now to be considered as a functional of $\tilde{S}(x)$ and $g(x)$,

$$\mathcal{A} = \int_{t_1}^{t_2} dt \left\{ i \int_{-\infty}^{\infty} dx \tilde{S}(x) \dot{g}(x) - \bar{H}[g, \tilde{S}] \right\}. \quad (5.32)$$

(iii) ECCM. It is permissible to continue to use the same expression for $\bar{U}$ as for the NCCM in Eq. (5.31), but now to consider the functions $\tilde{S}_F(q)$ and $B(u, q)$ to be functionals of $\tilde{S}(x)$ and $\gamma(x)$. For explicit forms of U we may always use the series expression (5.22). We thus obtain the ECCM expression

$$\bar{H} = \frac{1}{2} + \int_{-\infty}^{\infty} dx \tilde{S}'(x) x \gamma(x) + \int_{-\infty}^{\infty} \frac{dq}{2\pi} \tilde{S}_F(q) U(iq + u + \partial_u) e^{B(u,q)}|_{u=0}, \quad (5.33)$$

and the action in the ECCM case is given as

$$\mathcal{A} = \int_{t_1}^{t_2} dt \left\{ i \int_{-\infty}^{\infty} dx \tilde{S}(x) \dot{\gamma}(x) - \bar{H}[\gamma, \tilde{S}] \right\}. \quad (5.34)$$

These expressions for the action in the various IC parametrizations now permit a variational determination of the corresponding amplitudes and their dynamical evolution, as explained in the general case in Section II. A fuller discussion of the various functional derivatives involved is given in the subsequent paper (II), together with some illustrative examples.

VI. SUMMARY AND DISCUSSION

It should be clear from our discussion that the use of the holomorphic representations in their respective Bargmann Hilbert spaces of the model field theories under study, has enabled us fully to algebraize each of the three IC parametrizations. For example, we have demonstrated how the linked-cluster amplitudes $\{s_n\}$ and $\{\sigma_n\}$ may be constructed as the moments of specific generalized functions or Schwartz distributions, which themselves depend on the distribution of the zeros of the holomorphic wave function $F(z)$.

Furthermore, we have shown how an average-value generating functional can be constructed for each IC parametrization so that the various IC amplitudes $\{x_n, \tilde{x}_n\}$ need never explicitly appear. Instead, they can be eliminated in favour of the corresponding complex functions $\{X(z), \tilde{X}(z)\}$ and their Fourier transforms. In this way we have shown how the various formally divergent expansions in terms of the CC coefficients can be given a precise but not necessarily unique interpretation. The exact mappings of the original quantum field theory in its Hilbert space into a corresponding multiconfigurational classical field theory, which are provided by all three IC parametrizations, are thereby seen to be one-to-many mappings in the case of the nonlinear CC parametrizations. One of the main outcomes of our study has been to give what we believe to be the most complete analysis for any nontrivial model field theory of the asymptotic structure of the various amplitudes which fully and exactly characterize it.

In practical implementations of any of the three IC parametrizations one needs to approximate by restricting the general set of configurations $\{I\}$, and the corresponding set of operators $\{C_I^\dagger, C_I\}$ which completely span the original Hilbert space, to some subset. A very natural hierarchy of approximations is provided by the so-called SUB(N) scheme in which the respective configuration coefficients $\{x_I, \tilde{x}_I\}$ are truncated at the level where the general set-index $\{I\}$ contains no more than N single-particle (or, for fermions, single pairs of particle-hole) labels. For our simple model field theories considered here, the various complete sets of coefficients $\{x_n, \tilde{x}_n\}$ are truncated in SUB(N) approximation by retaining only those parameters with index $n \leq N$. In this way the various analytic functions $\{X(z), \tilde{X}(z)\}$ are approximated by N th-order polynomials.

For example, in the NCCM the operator $F(z)$ is replaced in the SUB(N) approximation by a function $F_{(N)}(z) = \exp[S_{(N)}(z)]$, where $S_{(N)}(z)$ is a polynomial of order N . From the discussion in Appendix A it is clear that the corresponding approximated wave functions $F_{(N)}(a^\dagger)|0\rangle$ coincide with ordinary Glauber coherent states when $N=1$ and with squeezed coherent states when $N=2$ (and $|s_2| < \frac{1}{2}$). These latter states are often called one-photon and two-photon coherent states in the context of quantum optics with a single-mode laser field, for example. Our corresponding states with $N>2$ may clearly be regarded in this context as N -photon (hypersqueezed) coherent states, or in general as multicoherent (or supercoherent) states. In the broader setting of quantum field theory, the NCCM SUB(N) approximations with $N>2$ may be regarded as a systematic means to go

beyond some appropriate Gaussian (or Bogoliubov) approximation. Although we may certainly obtain finite and perfectly well-defined expressions for energies and average values of other operators with such approximate NCCM states with $N > 2$, it is clear that these states have infinite norm and hence do not belong to the original Hilbert space $\mathcal{H}$.

Such SUB(N) hierarchies for the CC parametrizations therefore necessarily involve us in excursions out of $\mathcal{H}$. It is clear that there are hazards involved in such schemes, and their behaviour as $N \rightarrow \infty$ is not obvious. In terms of the holomorphic representation it is clear that whereas the exact $F(z)$ is an entire function of order two, it is replaced in the NCCM SUB(N) approximation by the entire function $F_{(N)}(z)$ of order N whose asymptotic behaviour is proportional to $\exp(s_N z^N)$. In the CC methods the physically important region for all expectation values, for example, is the vicinity of the origin. Whereas such SUB(N) approximations are (designed to be) excellent approximations to the exact functions in this region, their asymptotic behaviour is clearly seriously in error. In this way we may understand both why the SUB(N) scheme for the CC parametrizations can suffer from such seemingly serious flaws as lack of normalizability and yet can be extremely accurate in practice, even at very low levels of truncation, as has been demonstrated many times in applications to real physical systems [1].

One of the reasons for the great accuracy of the CCM parametrizations, compared with their CIM counterpart at comparable levels N of SUB(N) truncation for real many-body systems, is the increased degree of incorporation of the full locality and separability aspects of an exact description. In terms of the amplitudes $\{x_n, \tilde{x}_n\}$ this is usually described diagrammatically via their various connectivity properties. In order to make such diagrammatic expansions in terms of these amplitudes, it is necessary in principle to consider their convergence properties. What we have shown explicitly here is how the formally divergent series that certainly appear in the CCM cases, can be regularized or given meaning in an exact and well-defined fashion. We leave it to a subsequent paper (II) to focus on these diagrammatic topological connectivity properties, and on the related structure of the associated classical phase spaces induced by each IC parametrization. We also defer until then a discussion of the possible extensions of the holomorphic formalism developed here for model field theories with a single-mode creation operator $a^\dagger$, and hence having a Bargmann Hilbert space of a single complex variable z , to the more physical cases of local continuum quantum field theories in d dimensions, where $a^\dagger \rightarrow a^\dagger(\vec{x})$ and $\vec{x}$ is a d -dimensional vector.

APPENDIX A: COHERENT AND RELATED SQUEEZED STATES

We have seen how the ground-state wave function $|0\rangle$ of the harmonic oscillator (HO) Hamiltonian of Eq. (3.5) may be used as the cyclic vector in the Fock space defined with respect to the corresponding operators a and $a^\dagger$ of Eq. (3.2),

$$a|0\rangle = 0. \tag{A1}$$

The Glauber coherent states $|z\rangle$ are similar defined to be the eigenstates of the destruction operator a ,

$$a|z\rangle = z|z\rangle; \quad z \in \mathbb{C}. \quad (\text{A2})$$

A complete set of ket states in this Fock space is the orthonormal basis $\{|n\rangle\}$ of eigenstates to the HO Hamiltonian of Eq. (3.5),

$$|n\rangle = (n!)^{-1/2} (a^\dagger)^n |0\rangle; \quad n = 0, 1, 2, \dots \quad (\text{A3})$$

By expanding $|z\rangle$ in this basis it is simple to show from the basic commutation relation of Eq. (3.3) that the (normalized) coherent state is given as

$$\begin{aligned} |z\rangle &= e^{-|z|^2/2} \sum_{n=0}^{\infty} \frac{z^n}{n!} (a^\dagger)^n |0\rangle \\ &= e^{-|z|^2/2} e^{za^\dagger} |0\rangle, \end{aligned} \quad (\text{A4})$$

and where the explicit normalization, $\langle z|z\rangle = 1$, follows trivially from Eq. (3.8). By making use of the Baker–Campbell–Hausdorff relation,

$$e^{\lambda a + \mu a^\dagger} = e^{\lambda a} e^{\mu a^\dagger} e^{-\lambda\mu/2} = e^{\mu a^\dagger} e^{\lambda a} e^{\lambda\mu/2}, \quad (\text{A5})$$

it is also easy to express $|z\rangle$ as a unitary operator acting on the vacuum $|0\rangle$,

$$|z\rangle = \exp(za^\dagger - z^*a) |0\rangle. \quad (\text{A6})$$

By making use of Eqs. (A4) and (3.8), it is easy to derive the overlap relation,

$$\langle z|z'\rangle = \exp\left(-\frac{1}{2}|z|^2 - \frac{1}{2}|z'|^2 + z^*z'\right), \quad (\text{A7})$$

between any two coherent states. Furthermore, by taking matrix elements between arbitrary members $|n\rangle$ and $\langle m|$ of the complete basis (A3), one may readily show using Eqs. (A2) and (3.12) that a resolution of the identity operator can be given in terms of the (over-)complete set of coherent states as

$$\mathbb{1} = \frac{1}{\pi} \int d^2z |z\rangle \langle z|. \quad (\text{A8})$$

The Schrödinger wave function of the Glauber coherent state, $\psi_z(x) \equiv \langle x|z\rangle$ is readily obtained from Eq. (A4) and the decomposition of Eq. (3.2),

$$\langle x|z\rangle = e^{-|z|^2/2} \exp\left[\frac{z}{\sqrt{2}}\left(x - \frac{d}{dx}\right)\right] \langle x|0\rangle. \quad (\text{A9})$$

The further use of the Baker–Campbell–Hausdorff theorem gives

$$\langle x|z\rangle = \exp\left(-\frac{1}{2}|z|^2 - \frac{1}{4}z^2 + zx/\sqrt{2}\right) \langle x - z/\sqrt{2}|0\rangle, \quad (\text{A10})$$

and hence from Eq. (3.7) the final relation,

$$\psi_z(x) \equiv \langle x|z\rangle = \pi^{-1/4} \exp(-\tfrac{1}{2}|z|^2 - \tfrac{1}{2}z^2 + \sqrt{2}xz - \tfrac{1}{2}x^2). \quad (\text{A11})$$

It is clear from Eq. (A11) that the state $|z\rangle$ is related to the vacuum state $|0\rangle$ by a simple shift or displacement of the origin in the coordinate-space or Schrödinger representation, by an amount $\sqrt{2}z$. It is also trivial to verify that Eq. (A11) satisfies the normalization condition,

$$\langle z|z\rangle = \int_{-\infty}^{\infty} dx |\psi_z(x)|^2 = 1. \quad (\text{A12})$$

We now consider a more general harmonic oscillator centered at x_0 and with an arbitrary width parameter α . Its Hamiltonian is thus specified as

$$H^0(x_0, \alpha) = \frac{1}{2}\alpha^2\hat{p}^2 + \frac{(\hat{x} - x_0)^2}{2\alpha^2}. \quad (\text{A13})$$

By comparison with our original Hamiltonian, $H^0 = H^0(0, 1)$, of Eq. (3.5), the HO potential (A13) is both displaced or shifted (by an amount x_0), and scaled or squeezed by an amount which is determined by α (i.e., $\alpha < 1$ gives "squeezing," and $\alpha > 1$ gives "anti-squeezing" in the x -coordinate). The ground-state wave function $|x_0, \alpha\rangle_0$ of $H^0(x_0, \alpha)$ has eigenvalue $\frac{1}{2}$ and coordinate-space representation given by the usual Gaussian form,

$$\begin{aligned} \psi_{x_0, \alpha}^0(x) &\equiv \langle x|x_0, \alpha\rangle_0 \\ &= \frac{1}{\alpha} (2\pi)^{-1/2} \exp\left[-\frac{(x - x_0)^2}{2\alpha^2}\right], \end{aligned} \quad (\text{A14})$$

where we have now chosen the convenient but non-standard normalization such that

$$\int_{-\infty}^{\infty} dx \psi_{x_0, \alpha}^0(x) = 1. \quad (\text{A15})$$

This difference in normalization ensures that $|0, 1\rangle_0$ and $|0\rangle$ differ by an overall multiplicative constant. We note that in the extreme squeezing limit, $\alpha \rightarrow 0$,

$$\lim_{\alpha \rightarrow 0} \psi_{x_0, \alpha}^0(x) = \delta(x - x_0) = \langle x|x_0\rangle, \quad (\text{A16})$$

and we simply obtain the position eigenstate $|x_0\rangle$,

$$\hat{x}|x_0\rangle = x_0|x_0\rangle. \quad (\text{A17})$$

It is of particular interest for present purposes to write the state $|x_0, \alpha\rangle_0$ in the Fock-space representation characterized by the ladder operators a and $a^\dagger$ of Eq. (3.2) for the undisplaced ($x_0 = 0$) and unsqueezed ($\alpha = 1$) original HO potential of Eq. (3.5). We write its CIM representation in the form

$$|x_0, \alpha\rangle_0 \equiv G(a^\dagger)|0\rangle. \quad (\text{A18})$$

The holomorphic wave function $G(z)$ is then found in terms of the corresponding Schrödinger wave function $\psi_{x_0, \alpha}^0(x)$ of Eq. (A14) from the general relation (3.29). In this way we readily obtain

$$|x_0, \alpha\rangle_0 = \pi^{-1/4} (1 + \alpha^2)^{-1/2} \exp(Aa^{\dagger 2} + Ba^{\dagger} + C) |0\rangle, \quad (\text{A19})$$

where the constants A , B , and C are given as

$$A \equiv -\frac{1}{2} \left(\frac{1 - \alpha^2}{1 + \alpha^2} \right); \quad B \equiv \frac{\sqrt{2} x_0}{(1 + \alpha^2)}; \quad C \equiv -\frac{x_0^2}{2(1 + \alpha^2)}. \quad (\text{A20})$$

We clearly observe that such squeezed (and displaced) Gaussian states have a natural NCCM representation in terms of a holomorphic function $S(z)$ of quadratic form, $S(z) = Az^2 + Bz$, whereas the Glauber coherent states had an NCCM representation in which $S(z)$ is linear. It is also clear that states of the general form (A19) are normalizable only when $|A| < \frac{1}{2}$. In such cases they also may be written, by analogy with Eq. (A6) as a unitary operator acting on the vacuum $|0\rangle$, although we do not explicitly construct it here. In the limit that $A \rightarrow -\frac{1}{2}$ we obtain the position eigenstate from Eq. (A16) in the form,

$$\begin{aligned} |x_0\rangle &= \lim_{\alpha \rightarrow 0} |x_0, \alpha\rangle_0 \\ &= \pi^{-1/4} e^{-x_0^2/2} \exp\left(-\frac{1}{2}a^{\dagger 2} + \sqrt{2}x_0a^{\dagger}\right) |0\rangle. \end{aligned} \quad (\text{A21})$$

By using the representation of Eq. (3.2), one can check directly that the explicit state of Eq. (A21) does indeed satisfy the eigenvalue relation of Eq. (A17).

We note in passing that the squeezed and displaced harmonic oscillator ground state $|x_0, \alpha\rangle_0$ may itself also be associated with a destruction operator b which annihilates it, just as the destruction operator a annihilates the unsqueezed state $|0\rangle$. The mapping between the operators $(b, b^{\dagger})$ and $(a, a^{\dagger})$ is a canonical one, and is just the usual linear Bogoliubov transformation, including an inhomogeneous (c -number) term to account for the displacement. The so-called Gaussian or Hartree variational approximation for the full AO problem amounts to an optimal choice for the parameters x_0 and α in the sense of minimizing the expectation value of the AO Hamiltonian over the class of trial states $\{|x_0, \alpha\rangle_0\}$.

Finally, we also note that the inner product between any two such (normalizable) squeezed states as given by Eq. (A19) is readily obtained using the general relation (3.13). We obtain the useful result,

$$\langle 0 | e^{Aa^2 + Ba e^{Ca^{\dagger 2}} + Da^{\dagger}} | 0 \rangle = (1 - 4AC)^{-1/2} \exp\left(\frac{AD^2 + B^2C + BD}{1 - 4AC}\right). \quad (\text{A22})$$

APPENDIX B: THE ANALYTIC FUNCTIONS $\psi_0(z)$ AND $F^0(z)$

The analytic properties of both the ground-state wave function ψ_0 of the anharmonic oscillator (AO) potential of Eqs. (3.31) and (3.32), and its holomorphic

representation F^0 , are now studied using the lowest-order WKB method. Although this method is certainly not mathematically definitive in the sense of being completely rigorous, the results of using it are sufficiently reliable and accurate to be useful in our analysis of the CC parametrizations. In particular, we have not discovered a rigorous analysis of the WKB method for differential equations of higher than second order. Our discussion of $F^0(z)$ will hence be restricted to a rather straightforward generalization of the standard method (see, e.g., Ref. [47]).

Let the analytic continuation $\psi_0(z)$ off the real axis of the wave function $\psi_0(x)$ be represented in the WKB form,

$$\psi_0(z) = e^{Q(z)}. \quad (\text{B1})$$

In order to satisfy the differential equation (3.32), one must have the asymptotic behaviour,

$$Q(z) \xrightarrow{|z| \rightarrow \infty} \pm az^{K+1}, \quad (\text{B2})$$

where $a \equiv \sqrt{\lambda}/(K+1)$. The general solution is then the superposition of the two WKB solutions,

$$\psi_0(z) = A(z) \exp(az^{K+1}) + B(z) \exp(-az^{K+1}), \quad (\text{B3})$$

which expression is to be properly interpreted in the WKB sense. Thus, the coefficients $A(z)$ and $B(z)$ are functions of z which are of order unity and slowly varying in comparison with the exponential WKB factors, as $|z| \rightarrow \infty$. Furthermore, one or the other of the coefficient functions A and B may also be asymptotically precisely zero in certain directions from the origin along lines on which the WKB exponents are real, called the Stokes lines.

Furthermore, a set of anti-Stokes lines also exists, on which the exponent $Q(z)$ is imaginary. These lines divide the complex z -plane into the $2(K+1)$ sectors $\{\mathbb{S}_n\}$,

$$\mathbb{S}_n: \frac{(2n-1)\pi}{2(K+1)} \leq \arg z \leq \frac{(2n+1)\pi}{2(K+1)}; \quad n = 0, 1, \dots, 2K+1. \quad (\text{B4})$$

The dominant solution in the sector $\mathbb{S}_n$ in the asymptotic region $|z| \rightarrow \infty$ is the first term in Eq. (B3) with coefficient A for even values of n , and the second term with coefficient B for odd values of n . The dominant term is generally nonzero in each sector, but due to the unidirectional nature of the WKB connection formulae the coefficient of the dominant term in sector $\mathbb{S}_n$ cannot be connected to the coefficient of the same term in sector $\mathbb{S}_{n+2}$ across the intervening sector $\mathbb{S}_{n+1}$ wherein the other term dominates.

Nevertheless, the normalizability of ψ_0 imposes two extra conditions. Thus, along the positive real axis (which is a Stokes line) in sector $\mathbb{S}_0$ one must have $A \rightarrow 0$ as $x \rightarrow +\infty$, and along the negative real axis in sector $\mathbb{S}_{K+1}$ one must have either $A \rightarrow 0$ (for odd K) or $B \rightarrow 0$ (for even K) as $x \rightarrow -\infty$. Even with these restrictions, the WKB connection formulae cannot normally prevent the dominant term from being nonzero in all of the others sectors. In the middle of these sectors, around the

Stokes lines, $|\psi_0(z)|$ is therefore large, whereas on the boundaries between them, namely the anti-Stokes lines, $\psi_0(z)$ develops zeros due to interference. It is then not difficult to calculate that the zeros $\{z_m^\phi\}$ of the wave function, $\psi_0(z_m^\phi) = 0$, are expected to be asymptotically located at the points

$$z_m^\phi \xrightarrow{m \rightarrow \infty} \eta \rho m^{1/(K+1)}; \quad \rho = \left[\frac{(K+1)\pi}{\sqrt{\lambda}} \right]^{1/(K+1)}, \quad (\text{B5})$$

where $\eta = e^{i\phi}$, and the angle ϕ may be any of the $2(K-1)$ values,

$$\phi = \pm \frac{(2n+1)\pi}{2(K+1)}; \quad n = 1, 2, \dots, K-1. \quad (\text{B6})$$

In particular, this asymptotic distribution of zeros specified by Eqs. (B5) and (B6) agrees with the well-known result [48] that the zeros of $\psi_0(z)$ for the quartic ($K=2$) anharmonic oscillator lie on the imaginary axis.

We stress that the derived results of Eqs. (B5) and (B6) represent the *maximum possible* number of zeros. In this respect they are in agreement with the general theorems [49] concerning the maximum density of zeros of entire functions of order $(K+1)$. However, since $\psi_0(z)$ is an entire function of *integral* order, the number of zeros may actually be reduced in specific cases. For example, the entire function $\psi(z) = \exp(-z^{2l}/2l)$ has *no* zeros but is the ground-state wave function for the potential $V(z) = \frac{1}{2}z^{4l-2} - (l - \frac{1}{2})z^{2l-2}$.

If we now turn our attention to the holomorphic wave function $F^0(z)$ corresponding to the AO wave function ψ_0 , and write it in the form

$$F^0(z) = \exp(-\frac{1}{2}z^2)f^0(z), \quad (\text{B7})$$

then the factor function $f^0(z)$ satisfies the differential equation (3.34). If $f^0(z)$ is also represented in the WKB form

$$f^0(z) = e^{T(z)}, \quad (\text{B8})$$

then Eq. (3.34) shows that asymptotically as $|z| \rightarrow \infty$, $T(z)$ must behave as one of the $2K$ solutions $\{T_{(n)}(z)\}$,

$$T_{(n)}(z) = \varepsilon^n b z^\nu; \quad n = 0, 1, \dots, 2K-1, \quad (\text{B9})$$

where

$$\nu \equiv \left(\frac{K+1}{K} \right); \quad \varepsilon = \exp\left(i \frac{\pi}{K}\right); \quad b \equiv \frac{1}{\nu} \left(\frac{2^{K+1}}{\lambda} \right)^{1/(2K)}. \quad (\text{B10})$$

To be specific we choose the branch cut of z^ν in Eq. (B9) to be the negative real axis. The full solution to Eq. (3.34) is now written as the superposition,

$$f^0(z) = \sum_{n=0}^{2K-1} a_n(z) \exp[T_{(n)}(z)], \quad (\text{B11})$$

where the coefficient functions $a_n(z)$ are once again relatively slowly varying functions of z in comparison with the WKB solutions. The various branches of f^0 must now be matched in a way which both satisfies the boundary conditions and is consistent with the unidirectional nature of the connection formulae in WKB theory.

The requirement of normalizability for $F^0(z)$ ensures from Eq. (3.13) that the function $\exp(-|z|^2) |F^0(z)|^2$ is integrable over the entire complex plane. Hence on lines parallel to the imaginary axis, one must have (for $x, y \in \mathbb{R}$) $|f^0(x + iy)| \rightarrow o(1)$ as $y \rightarrow \pm\infty$. Since $f(z)$ is a real analytic function (i.e., real on the real axis) which is also even, we may initially focus on its behaviour in the first quadrant, namely $0 \leq \arg(z) \leq \frac{1}{2}\pi$. Of the $2K$ terms in the sum in Eq. (B11), those with $n = K, K+1, \dots, 2K-1$ are asymptotically large as $y \rightarrow +\infty$, and the corresponding coefficients a_n must therefore asymptotically vanish. Thus, in the first quadrant of the complex plane only the branches with $n = 0, 1, \dots, K-1$ are allowed as asymptotic forms. It is easy to see that of these allowed solutions the $n=0$ branch is actually asymptotically dominant everywhere in the first quadrant. A similar analysis in the fourth quadrant, namely, $-\frac{1}{2}\pi \leq \arg(z) < 0$, shows that only the terms in Eq. (B11) with $n=0$ or $n = K+1, K+2, \dots, 2K-1$ are allowed as asymptotic forms. Once again, it is readily observed that of these allowed branches, the $n=0$ branch is asymptotically dominant everywhere in the fourth quadrant. We discover in this way that the leading branch in the entire right half-plane; $-\frac{1}{2}\pi < \arg(z) < \frac{1}{2}\pi$ is the $n=0$ branch. Using the even symmetry of $f^0(z)$, our final result for the asymptotic behaviour of $f^0(z)$ is expressed as

$$f^0(z) \xrightarrow{|z| \rightarrow \infty} \begin{cases} \exp(bz^v), & \operatorname{Re} z > 0, \\ \exp[b(-z)^v], & \operatorname{Re} z < 0 \end{cases} \quad (\text{B12})$$

where b and v are as given in Eq. (B10).

A result of the above analysis is that only the imaginary axis remains as a boundary where branches of equal magnitude destructively interfere (i.e., an anti-Stokes line). The zeros are then easily found to be located asymptotically at the points z_m , $f^0(z_m) = 0$, where

$$z_m \xrightarrow{m \rightarrow \infty} \pm iy_m; \quad y_m = \rho' m^{1/v}, \quad (\text{B13})$$

$$\rho' = \left[\frac{\pi}{b} \sec\left(\frac{\pi}{2K}\right) \right]^{1/v}.$$

It is interesting to verify this result in the exactly soluble limit $K \rightarrow \infty$, which corresponds to the infinite square-well potential,

$$V(x) = \begin{cases} 0, & |x| < 1 \\ \infty, & |x| > 1. \end{cases} \quad (\text{B14})$$

In this case the ground-state wave function is simply given as $\psi_0(x) =$

$\theta(1-x^2) \cos(\frac{1}{2}\pi x)$. The corresponding holomorphic wave function $F^0(z)$ is given by the integral representation of Eq. (3.29). By analyzing the variations of sign of $F^0(iy)$ in this case as $y \rightarrow \infty$ it can readily be seen that the asymptotic result is that the zeros become equally spaced along the imaginary axis, $y_m \rightarrow m\pi/\sqrt{2}$ as $m \rightarrow \infty$. This result agrees precisely with that obtained from the general result of Eq. (B13) in the limit $K \rightarrow \infty$.

APPENDIX C: THE AO FUNCTION $\tilde{S}^0(z)$

In order to study the analytic properties of the NCCM function $\tilde{S}^0(z)$ for the AO ground state, we use the integral representation of Eq. (4.11). For ease of notation we denote $u \equiv z/\sqrt{2}$, and write $\psi_0(z)$ in the WKB form of Eq. (B1). Thus,

$$\tilde{S}^0(z) = \frac{1}{N^2} e^{-z^2/2} \Omega(z/\sqrt{2}), \quad (C1)$$

where the normalization factor N^2 is as given in Eq. (3.24) and where

$$\Omega(u) \equiv \int_{-\infty}^{\infty} dx \exp[xu + Q(x) + Q(x-u)]; \quad u \in \mathbb{C}. \quad (C2)$$

For the AO systems of order $2K (\geq 2)$ under consideration, the function $Q(z)$ vanishes so rapidly for $\text{Re } z \rightarrow \pm\infty$, as can be seen from Eq. (B2), that the integral in Eq. (C2) converges for arbitrary values of u . Hence, $\tilde{S}^0(z)$ is an entire function. We now proceed to demonstrate that it is an entire function of the same order, namely $(K+1)$, as $\psi_0(z)$. For that purpose it is quite sufficient to estimate the asymptotic behaviour of $\Omega(u)$ as $|u| \rightarrow \infty$ in some suitably chosen direction. In what follows below we use the saddle-point method, and restrict ourselves very specifically to the cases $K = 3, 7, 11, \dots$. The results are qualitatively similar for other values of K , although the particular details of the proof differ.

In the first place we consider $u = iv$, where v is real and positive, and let $v \rightarrow \infty$. The stationary points of the exponent function in Eq. (C2),

$$\Theta(x) \equiv xu + Q(x) + Q(x-u), \quad (C3)$$

are then found to be at the points

$$x_s \xrightarrow[v \rightarrow \infty]{} \frac{v}{2 \sin \theta_s} e^{i\theta_s} + \frac{i}{2K\sqrt{\lambda}} \left(\frac{v}{2 \sin \theta_s} \right)^{2-K}; \quad s = 1, 2, \dots, K, \quad (C4)$$

where

$$\theta_s = \frac{\pi}{2K} (2s-1); \quad s = 1, 2, \dots, K. \quad (C5)$$

We readily observe that each such stationary point x_s in the limit $v \rightarrow \infty$ is in the corresponding sector $\mathbb{S}_s$ defined in Eq. (B4). At these points $\{x_s\}$, the exponent function $\Theta(x)$ has a negative second derivative, $\Theta''(x_s) < 0$, so that $\Theta(x_s)$ is a local maximum on a line parallel to the real axis passing through x_s . The dominant saddle points are the two points x_1 and x_K . They yield a contribution to $\Omega(iv)$ given by

$$\Omega(iv) \xrightarrow{v \rightarrow \infty} \exp(cv^{K+1}), \quad (\text{C6})$$

where the constant c is given as

$$c = \frac{\sqrt{\lambda}}{2^K(K+1)} \left[\operatorname{cosec} \left(\frac{\pi}{2K} \right) \right]^K. \quad (\text{C7})$$

We do not pursue the study of the asymptotic behaviour of $\Omega(u)$, and hence $\tilde{S}^0(z)$, in other general directions in the complex plane, since the results are qualitatively similar. Nevertheless, it is interesting to consider the behaviour along the real axis as a special case. For large real values of u there is a unique maximum for the function $\Theta(x)$ at the point x_0 , where

$$x_0 \xrightarrow{u \rightarrow +\infty} \frac{1}{2}u + \frac{1}{K\sqrt{\lambda}} \left(\frac{2}{u} \right)^{K-2}. \quad (\text{C8})$$

The value of $\Theta(x)$ at this point is

$$\Theta(x_0) \approx -\frac{2\sqrt{\lambda}}{(K+1)} \left(\frac{1}{2}u \right)^{K+1}, \quad (\text{C9})$$

from which it is found that the asymptotic behaviour along the positive real axis of $\tilde{S}^0(z)$ is given by

$$\tilde{S}^0(x) \xrightarrow{x \rightarrow \infty} \exp \left(-\frac{\sqrt{\lambda}}{(K+1)} 2^{-(3K+1)/2} x^{K+1} \right). \quad (\text{C10})$$

We note finally that Eqs. (4.13a) and (4.14) provide a very convenient formal representation of the operator $\tilde{S}(a)$ as

$$\tilde{S}(a) = \int_{-\infty}^{\infty} \frac{dq}{2\pi} \tilde{F}_F(q) F(iq) e^{iq a}, \quad (\text{C11})$$

in the normalization scheme where

$$\langle 0 | \tilde{F} F | 0 \rangle = \int_{-\infty}^{\infty} \frac{dq}{2\pi} \tilde{F}_F(q) F(iq) = 1. \quad (\text{C12})$$

In the NCCM parametrization, for example, the bra states in $\mathcal{H}$ are thus represented as,

$$\langle 0 | \tilde{S}(a) \frac{1}{F(a^\dagger)} = \langle 0 | \left(\int_{-\infty}^{\infty} \frac{dq}{2\pi} \tilde{F}_F(q) F(iq) e^{iqa} \frac{1}{F(a^\dagger)} \right). \quad (\text{C13})$$

By making use of the elementary relation,

$$e^{iqa} a^\dagger e^{-iqa} = a^\dagger + iq, \quad (\text{C14})$$

and the definition $\langle 0 | a^\dagger = 0$ of the vacuum state $\langle 0 |$, we have

$$\langle 0 | e^{iqa} [F(a^\dagger)]^{-1} = [F(iq)]^{-1} \langle 0 | e^{iqa}. \quad (\text{C15})$$

Insertion of Eq. (C15) into Eq. (C13) yields the required result,

$$\langle 0 | \tilde{S}(a) \frac{1}{F(a^\dagger)} = \langle 0 | \left(\int_{-\infty}^{\infty} \frac{dq}{2\pi} \tilde{F}_F(q) e^{iqa} \right) \equiv \langle 0 | \tilde{F}(a). \quad (\text{C16})$$

Clearly the factor $1/F(a^\dagger)$ in Eq. (C13) is highly singular, and hence of dubious interpretation as a linear operator, since it has poles of first order in its argument. Nevertheless, in expressions for average values, for example, it always appears bracketed from the left by the operator $\tilde{S}(a)$, which has in its Fourier transform zeros at precisely the same places, so that the poles of $1/F$ are cancelled. Exactly the same argument applies to the generating functional for average values, so that it too is mathematically well defined.

APPENDIX D: PROOF OF THE DIVERGENCE OF EQ. (4.29)

The formal expansion for the ECCM coefficients $\{\sigma_n\}$ in terms of the complete set of NCCM coefficients $\{s_n, \tilde{s}_n\}$ is given by Eq. (4.29) as

$$\sigma_n = \sum_{m=0}^{\infty} a_{nm}; \quad a_{nm} = \frac{(m+n)!}{n!} \tilde{s}_m s_{m+n}. \quad (\text{D1})$$

In order to examine the convergence properties of this series we need to know the asymptotic behaviour of the coefficients $\{a_{nm}\}$ as $m \rightarrow \infty$, and hence also of the NCCM coefficients. For the amplitudes $\{s_m\}$ we have from Eq. (4.21),

$$|s_m| \propto \frac{1}{m} \rho^{-m}; \quad m \rightarrow \infty, \quad (\text{D2})$$

for some finite value of ρ . The corresponding behaviour of the coefficients $\{\tilde{s}_m\}$ is

readily obtained from the general theorem [49] that a necessary and sufficient condition that

$$H(z) = \sum_{m=0}^{\infty} h_m z^m \quad (\text{D3})$$

should be an integral function of (finite) order κ is that

$$\liminf_{m \rightarrow \infty} \frac{\ln(1/|h_m|)}{m \ln m} = \frac{1}{\kappa}. \quad (\text{D4})$$

For the case of the AO ground state, we have already shown in Appendix C that $\tilde{S}^0(z)$ is an entire function of order $(K+1)$. Equation (D4) thus shows that the corresponding expansion coefficients $\{\tilde{s}_m\}$ behave asymptotically as

$$|\tilde{s}_m| \propto m^{-m/(K+1)}, \quad m \rightarrow \infty, \quad (\text{D5})$$

at least for an infinite subset of $m \in \mathbb{N}$. Therefore, for a sufficiently numerous subset of values m in the limit as $m \rightarrow \infty$, we have the asymptotic behaviour (for fixed n),

$$|a_{nm}| \propto m^{mK/(K+1) + \alpha} (\rho e)^{-m} \rightarrow \infty, \quad (\text{D6})$$

where α is a constant. Thus, the sum (D1) clearly cannot converge in the ordinary sense.

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