Independent-Cluster Parametrizations of Wave Functions in Model Field Theories. III. The Coupled-Cluster Phase Spaces and Their Geometrical Structure

J. S. ARPONEN

*Department of Theoretical Physics, University of Helsinki, Siltavuorenpenger 20 C,
P.O. Box 9, FIN-00014 University of Helsinki, Finland*

AND

R. F. BISHOP

*Department of Mathematics,
University of Manchester Institute of Science and Technology,
P.O. Box 88, Manchester M60 1QD, England*

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In this third paper of a series we study the structure of the phase spaces of the independent-cluster methods. These phase spaces are classical symplectic manifolds which provide faithful descriptions of the quantum mechanical pure states of an arbitrary system. They are “super-spaces” in the sense that the full physical many-body or field-theoretic system is described by a point of the space, in contrast to “ordinary” spaces for which the state of the physical system is described rather by the whole space itself. We focus attention on the normal and extended coupled-cluster methods (NCCM and ECCM). Both methods provide parametrizations of the Hilbert space which take into account in increasing degrees of completeness the connectivity properties of the associated perturbative diagram structure. This corresponds to an increasing incorporation of locality into the description of the quantum system. As a result the degree of nonlinearity increases in the dynamical equations that govern the temporal evolution and determine the equilibrium state. Because of the nonlinearity, the structure of the manifold becomes geometrically complicated. We analyse the neighbourhood of the ground state of the one-mode anharmonic bosonic field theory and derive the nonlinear expansion beyond the linear response regime. The expansion is given in terms of normal-mode amplitudes, which provide the best local coordinate system close to the ground state. We generalize the treatment to other nonequilibrium states by considering the similarly defined normal coordinates around the corresponding phase space point. It is pointed out that the coupled-cluster method (CCM) maps display such features as (an)holonomy, or geometric phase. For example, a physical state may be represented by a number of different points on the CCM manifold. For this reason the whole phase spaces in the NCCM or ECCM cannot be covered by a single chart. To account for this non-Euclidean nature we introduce a suitable pseudo-Riemannian metric structure which is compatible with an important subset of all canonical transformations. It is then shown that the phase space of the configuration-interaction method is flat, namely the complex Euclidean space; that the NCCM manifold has zero curvature even

though its Riemann tensor does not vanish; and that the ECCM manifold is intrinsically curved. It is pointed out that with the present metrization many of the dimensions of the ECCM phase space are effectively compactified and that the overall topological structure of the space is related to the distribution of the zeros of the Bargmann wave function. © 1993 Academic Press, Inc.

I. INTRODUCTION

For classical mechanical systems nonlinearity of the equations of motion is very much the norm. The study of such emergent phenomena as chaos which flow from the nonlinearity has largely been responsible for the huge recent revival of interest in classical mechanics. By contrast, quantum mechanics is a linear dynamical theory. As such, quantal systems are always formally integrable, and their temporal evolution can be interpreted as motion on a multi-dimensional (and usually infinite-dimensional) torus in some suitably defined phase space. The Hilbert space may hence always be envisaged as a complex Euclidean manifold.

In order to break away from the straitjacket that linearity seemingly imposes and to explore alternative possibilities, various attempts have been made to replace conventional quantum mechanics by some more general nonlinear theory. In a recent notable example [1, 2] suggested by Weinberg the starting point was the requirement of projectivity, whence the observables are invariant under multiplication of the wave function by an arbitrary constant. This requirement is implemented by introducing for the algebra of observables a particular star product which turns out to be non-associative, i.e., $a * (b * c) \neq (a * b) * c$. In order to test the possibility that such nonlinear terms may actually be required, the theory has been applied to the slowly driven hyperfine transition of ^9Be ions in an attempt to estimate the sensitivity of the resonance frequency to the change in occupation of the energy levels. Subsequent experiments (and see Ref. [3] for a review) detected no such detuning effects to a very high degree of accuracy. Another notable earlier attempt was due to Bialynicki-Birula and Mycielski [4], who modified the time-dependent Schrödinger equation by the introduction of a term involving the logarithm of the wave function. Although such a term preserves to some extent the physically intuitive separability properties of the system in the limit when it disintegrates into widely separated subsystems, the resulting theory is not projectively invariant in the above sense. It also leads to complications with regard to the normalization of the wave function and the zero-point of the energy scale. Furthermore, no experiments were found to verify this theory, either. Indeed, to date, *no* experimental results have been found which could not be explained by the conventional linear formalism.

Nevertheless, within various levels of *approximate* treatment of extended quantum-mechanical systems, nonlinear equations of motion do arise from within the underlying linear formalism. Hartree-Fock and other comparable mean field theory approximations are perhaps the most well known and simplest examples.

Variational approximations (of which mean-field theory is itself an example) also typically lead to nonlinear equations. Thus, without ever bringing into question the basic linear formulation of quantum mechanics, such approximations have the effect of smuggling nonlinearity into the history of events "by the back-door," as it were. In this way the possibility of chaotic behaviour, for example, is introduced, at least as far as the *local* properties of an extended system are concerned.

In geometrical terms, the introduction of nonlinear equations generally opens up the vista of a nontrivial structure for the space of the underlying dynamic variables [5]. Nevertheless, so long as the nonlinearity has itself only arisen from an *approximate* (e.g., mean-field) treatment of the otherwise exact quantum many-body or quantum field-theoretic correlations, any new emergent behaviour which arises from that nonlinearity retains an air of uncertainty. By contrast, in the present work we are concerned with such questions as whether, without leaving the confines of ordinary linear quantum mechanics, it is possible to find physically motivated (but, in principle, *exact*) nonlinear parametrizations that can themselves lead to phase spaces of physical dynamical variables which have an intrinsically non-Euclidean manifold structure.

The context of this investigation is that it has arisen as part of a wider study of the detailed mathematical structure of the so-called *coupled-cluster method* (CCM) of quantum many-body theory. In particular, the present paper forms the third in a series, the two earlier members of which [6, 7] are henceforth referred to as I and II, respectively. The CCM, or $\exp(S)$ method as it was originally known, was invented by Coester [8] in 1958. It has since been developed by many authors and applied to a large number of condensed matter and other systems of interest in physics and chemistry with great success. Recent reviews of the method and its applications are contained in Refs. [9, 10], and the interested reader is referred both to them and to our previous papers, I and II, for further references.

In brief, the CCM is a reformulation of standard (many-body) quantum mechanics. It therefore does not cast doubt on the linearity of the basic theory, although it is expressed in terms of nonlinear equations which satisfy both the separability and the projectivity requirements mentioned above. It is based on the fundamental observation that the quantum-mechanical wave function (especially for extended many-body or field-theoretic systems) is a global object with *multiplicative separability* properties with respect to fragmentation of the system into (widely separated) independent subsystems. The basic objects within the CCM are *additively separable* cluster amplitudes which are "local" quantities in the sense of obeying the usual cluster property [11]. In a suitable representation they are simply related to the *logarithm* of the wave function [8, 9]. The resulting coupled equations which determine these multi-configurational cluster amplitudes contain nonlinear combinations which explicitly preserve the connectivity properties of the related (Goldstone) diagrams. Furthermore, these properties are automatically preserved at any sensible level of truncation necessary for practical implementation. This latter feature is instrumental in guaranteeing the correct size-extensivity of quantities such as the total energy of the system. In this crucial respect for extended

systems, the CCM differs fundamentally from the simpler but related configuration-interaction method (CIM) [12] or generalized shell model.

Detailed comparisons between the CCM and the CIM in the above respects have been made elsewhere [13–15] by the present authors. More recent developments [16–18, 7] have pointed to the fact that the CCM introduces geometrical concepts such as an exactly mapped multi-configurational classical phase space which is a topologically nontrivial manifold. A detailed discussion of these *geometrical* aspects forms the core of this present work. It is in this main respect that it differs from the analysis in II which stressed the *algebraic* structure, and hence the local properties, of the CCM. In common with our earlier work in I and II, we again compare and contrast the two major variants of the CCM, namely the NCCM and ECCM versions [13], both with each other and with the CIM. As in I and II, we refer to these three methods generically as *independent cluster methods* (ICM).

The organization of the present article is as follows. In Section II we briefly summarize some of the main results concerning the supercoherent maps that each of the CIM, NCCM, and ECCM provides. These yield an *exact* “classicismation” mapping from the original quantum mechanics defined over a Hilbert space onto a symplectic differentiable manifold (namely, the classical ICM phase space) endowed with a classical Hamiltonian functional of the particular multi-configurational cluster amplitudes that characterize each method. As we have stressed elsewhere, especially the ECCM parametrization effects an exact correspondence between the global structure of a quantum state evolving with a linear dynamics in a Hilbert space, and the quasilocal structure of a set of (additively separable) cluster amplitudes evolving by a nonlinear classical dynamics in the multiconfigurational classical ECCM phase space.

In Section III we first consider a system (exemplified, as throughout our work, by a single-mode bosonic field theory) which is infinitesimally displaced away from its equilibrium ground state. We explicitly diagonalize the resulting second-order Hamiltonian functional which arises from this level of linear response, to obtain the normal modes. The displacements are then generalized to finite (i.e., non-infinitesimal) values in order to consider the general nonlinear response away from equilibrium. The aim here is to construct a chart on the CCM manifolds (and hence to investigate their global structure) in a larger region around the stable ground-state point. We demonstrate explicitly that the higher-order anharmonic matrix elements of the nonlinear mapped classical CCM Hamiltonian functionals can all be given in terms of convergent integral expressions. In this way we are able rigorously to prove the *existence* of the corresponding NCCM and ECCM phase spaces. This is the first such proof for any nontrivial infinite-dimensional Hilbert space. In Section IV we also prove the *completeness* of the CCM parametrizations by calculating the normal coordinates in the CCM phase spaces for arbitrary states mapped from the original Hilbert space.

In Section V we first point out that the map from the Hilbert space to the CCM phase spaces contains nontrivial features such as (an)holonomy, or geometric phase. The ICM manifolds are found to be connected, and a physical state may be

represented by a number of different representative points on them. Our earlier results are then used to study the local differential geometry of the NCCM and ECCM manifolds by investigating the connections between the local normal-coordinate parametrizations for neighbouring points. In this way we aim to study whether or not the CCM phase spaces are genuinely non-Euclidean. In particular, we introduce a natural metric on the CCM manifolds together with the usual definition of parallel transport in terms of the symmetric Levi-Civita affine connections. For each of the resulting CIM, NCCM, and ECCM Riemann manifolds we compute the Riemann tensor and associated scalar curvature. Since the spaces in question are "superspaces," the metric is in no way directly connected, for example, to such a familiar concept as the metric of the space-time in relativity theory.

As expected, the bilinear structure of the CIM Hamiltonian functional manifests itself in a trivial (i.e., flat or Euclidean) manifold. Somewhat surprisingly, perhaps, the NCCM manifold also has zero scalar curvature, although its full Riemann tensor does not vanish. Only the fully nonlinear ECCM mapping, for which *all* of the cluster amplitude coordinates are additively separable, has nonzero curvature. Finally, we point out that in our geometrization it may be possible to interpret the CCM phase spaces as containing multidimensional "necks" or "handles" in their geometry. In turn, these would lead to an effective compactification of many of the dimensions of the classical mapped CCM manifold, with the associated possibility that only a simpler submanifold structure is of greater physical relevance. Finally, in Section VI we summarize and discuss our results.

II. SUMMARY OF PREVIOUS ANALYSIS

We first present a brief summary of those results of our previous papers I and II which will be needed in the present work. As pointed out in Refs. [13, 19], the ICM equations of motion can be derived from the action principle by requiring the functional

$$\mathcal{A} \equiv \int_{t_1}^{t_2} dt \langle \tilde{\Psi}(t) | \left(i \frac{\partial}{\partial t} - H \right) | \Psi(t) \rangle = \mathcal{A}_0 - \int_{t_1}^{t_2} dt \bar{H} \quad (2.1)$$

to be stationary against independent variations of the bra and ket state vectors. The quantity $\mathcal{A}_0$ above is the temporal action, which is diagonalized by each of the three ICM parametrizations. In the application to the single-mode bosonic field theory we use the Bargmann representation, whence the bra and ket states, $\langle 0 | \tilde{f}(a)$ and $f(a^\dagger) | 0 \rangle$, become represented by the entire functions $\tilde{f}(z)$ and $f(z)$, respectively. Normalizability requires these functions to be of order $\rho \leq 2$ (in particular, they thus can be polynomials), and if $\rho = 2$, of type $\tau \leq \frac{1}{2}$. If we write $f(z) = \sum_0^\infty f_n z^n$, $g(z) = \sum_0^\infty g_n z^n$, the simplest form for the scalar product of such functions is

$$\langle f^* | g \rangle \equiv \langle 0 | f(a) g(a^\dagger) | 0 \rangle = f\left(\frac{d}{dz}\right) g(z) \Big|_{z=0} = g\left(\frac{d}{dz}\right) f(z) \Big|_{z=0} = \sum_{n=0}^{\infty} n! f_n g_n. \quad (2.2)$$

The scalar product can be expressed in a number of alternative ways, in particular through the Fourier transform of one of the functions, such as,

$$\langle f^* | g \rangle = \int_P \frac{d\zeta}{2\pi} f_F(\zeta) g(i\zeta); \quad f(z) = \int_P \frac{d\zeta}{2\pi} e^{i\zeta z} f_F(\zeta), \quad (2.3)$$

where P is a suitable contour in the complex plane.

For a Hamiltonian of the form $H(a^\dagger, a)$ the eigenvalue equations for the bra and ket states are then,

$$\tilde{f}_F^n(x) H\left(ix, i \frac{d}{dx}\right) = E_n \tilde{f}_F^n(x); \quad H\left(ix, -i \frac{d}{dx}\right) f^n(ix) = E_n f^n(ix), \quad (2.4)$$

in a rather self-evident notation. The (bi)orthonormality of the states is expressed by

$$\delta_{m,n} = \langle \tilde{\Psi}_m | \Psi_n \rangle = \int_{-\infty}^{\infty} \frac{dx}{2\pi} \tilde{f}_F^m(x) f^n(ix). \quad (2.5)$$

For the anharmonic oscillator of order $2K$, i.e., the Hamiltonian $H = \frac{1}{2}p^2 + \frac{1}{2}x^2 + kx^{2K}$, it was shown in Appendix A of II that the asymptotic properties of the Bargmann eigenfunctions are

$$r_n(z) \equiv \frac{f^n(z)}{f^0(z)}; \quad |r_n(ix)| \xrightarrow{x \rightarrow \infty} \text{const} \times \exp \left\{ -\frac{\varepsilon_n}{N(K)} x^{(1-K)/K} \right\}, \quad (2.6)$$

where $\varepsilon_n = E_n - E_0$, and $N(K)$ is a positive constant, (cf., Eq. (A.14) of II). This expression clearly approaches a constant (and the same is true also for $x \rightarrow -\infty$), since $K > 1$.

In the coupled cluster methods the wave functions $\tilde{\Psi}$ and Ψ (or $\tilde{f}(z)$ and $f(z)$) are not parametrized linearly. The operators (or functions, as they appear in the Bargmann representation) that are parametrized linearly are, in the NCCM,

$$s(z) = \ln \frac{f(z)}{f(0)}; \quad \hat{s}(z) = \frac{f(d/dz) \tilde{f}(z)}{f(d/dz) \tilde{f}(z)|_{z=0}}, \quad (2.7)$$

and in the ECCM,

$$\sigma(z) = \tilde{s}(d/dz) s(z) - \tilde{s}(d/dz) s(z)|_{z=0}; \quad \tilde{\sigma}(z) = \ln \tilde{s}(z). \quad (2.8)$$

We introduce the basis functions

$$\tilde{s}^{mn}(z) = f^n \left(\frac{d}{dz} \right) \tilde{f}^m(z) = \int_{-\infty}^{\infty} \frac{dx}{2\pi} e^{izx} \tilde{s}_{\text{F}}^{mn}(x), \quad (2.9)$$

which have the Fourier transforms

$$\tilde{s}_{\text{F}}^{mn}(z) \equiv \int_{-\infty}^{\infty} dx e^{-izx} \tilde{s}^{mn}(x) = \tilde{f}_{\text{F}}^m(z) f^n(iz). \quad (2.10)$$

On the basis of the normalization requirement, Eq. (2.5),

$$\tilde{s}^{mn}(0) = \delta_{m,n}. \quad (2.11)$$

We also derived in Appendix A of II the asymptotic behaviour,

$$\tilde{r}_{mn}(z) \equiv \frac{\tilde{s}^{mn}(z)}{\tilde{s}^{00}(z)} \xrightarrow{z \rightarrow \infty} \text{const} \times \exp \left\{ -\frac{\varepsilon_m + \varepsilon_n}{(K-1)\sqrt{2k}} 2^{1/2} (K-1) z^{1-K} \right\}. \quad (2.12)$$

The right-hand side approaches a constant, since $K > 1$.

As regards the function $s(z)$, whose Taylor-expansion coefficients are the original coupled-cluster amplitudes as introduced by Coester [8], we derived the representation

$$s(z) \equiv \int_{L'} dx e^{xz} \hat{s}(x); \quad \hat{s}(x) = \int_L \frac{dz}{2\pi i} e^{-xz} s(z) \quad (z \in L, x \in L') \quad (2.13)$$

which involves the "conjugate" integration contours L and L' . Although $s(z)$ is analytic on the line L , as long as this does not pass through a zero of $f(z)$, the Fourier transform $\hat{s}(x)$ is a regularized generalized function [20], with one special point at $x = 0$.

From Eq. (2.8) the ECCM function $\sigma(z)$ is now obtained in the form

$$\sigma(z) = \int_{-\infty}^{\infty} dx (e^{xz} - 1) \hat{\sigma}(x); \quad \hat{\sigma}(x) \equiv \hat{s}(x) \hat{s}(x), \quad (2.14)$$

where $\hat{\sigma}(x)$ is again a generalized function. However, $\sigma(z)$ is an entire function of order $\nu = (K+1)/K$. The remarkable feature is that it is a different entire function for each specific way that the line L bisects the set of zeros of the Bargmann wave function $f(z)$. The number of such different possibilities is at most countably infinite.

The expectation value in the CIM of an arbitrary operator $O(a^\dagger, a)$ is given in the form

$$\bar{O} = \int_{-\infty}^{\infty} \frac{dx}{2\pi} \tilde{f}_{\text{F}}(x) O\left(ix, -i \frac{d}{dx}\right) f(ix). \quad (2.15)$$

Correspondingly, the form which will be useful for present purposes in the NCCM is

$$\bar{O} = \int_{-\infty}^{\infty} \frac{dx}{2\pi} \tilde{s}_F(x) e^{-s(ix)} O\left(ix, -i \frac{d}{dx}\right) e^{s(ix)}. \quad (2.16)$$

In general it is more convenient to use the generating functionals of II, since they can easily be given directly in terms of the canonical field functions. Indeed, the pairs $(\hat{s}(x), \tilde{s}(x))$ in the NCCM and $(\hat{\sigma}(x), \tilde{\sigma}(x))$ in the ECCM were shown in II to obey canonical commutation rules under the Poisson bracket.

III. NORMAL-COORDINATE EXPANSION AROUND THE STATIONARY GROUND STATE IN THE ICM PARAMETRIZATIONS

It is very generally true that by considering small (i.e., infinitesimal) perturbations around the stationary ground state of a system, we may both uncover the eigenenergies (or, equivalently, eigenfrequencies) and eigenstates of the system and calculate its dynamical linear response to weak external probes. The dynamics of such small oscillations around a stationary point is governed by an effective Hamiltonian which may be obtained by linearizing the equations of motion. (For the various ICM parametrizations of the single-mode bosonic field theories under consideration here, these are the generic equations (2.7) of paper II.) The effective Hamiltonian is thus second order in the small deviations $\{\delta x_n(t), \delta \tilde{x}_n(t)\}$ away from the stationary ground state specified by the particular ICM amplitudes which we denote generically as $\{x_n^0, \tilde{x}_n^0\}$. The positive- and negative-frequency normal modes are then obtained by diagonalizing this second-order effective Hamiltonian in each case. In the specific case of the ECCM this procedure has been described very generally in Refs. [21, 18].

One of our main aims in the present section is now to carry this process of diagonalization through in full detail for the single-mode bosonic field theories under consideration and in the Bargmann-space representation of all three ICM parametrizations at the ground-state point.

We begin with the simplest ICM parametrization, namely the CIM, and we consider first an *arbitrary* state $|\Psi(t)\rangle$ (i.e., one not necessarily restricted to an infinitesimal displacement away from the stationary ground state $|\Psi_0\rangle$). In the Bargmann Hilbert space it is thus characterized by the CIM holomorphic functions,

$$\begin{aligned} f(z; t) &= \sum_{m=0}^{\infty} C_m(t) f^m(z), \\ \tilde{f}(z; t) &= \sum_{m=0}^{\infty} \tilde{C}_m(t) \tilde{f}^m(z). \end{aligned} \quad (3.1)$$

The normalization condition $\langle \tilde{\Psi}(t) | \Psi(t) \rangle = 1$, together with the orthogonality relations (2.5), now implies

$$N^2(t) \equiv \sum_{n=0}^{\infty} \tilde{C}_n(t) C_n(t) = 1. \quad (3.2)$$

This turns out naturally to be a conserved quantity. It is also a trivial matter to use Eq. (2.15), together with Eqs. (2.4)–(2.5), to derive the CIM expression,

$$\langle \tilde{\Psi}(t) | H | \Psi(t) \rangle = \bar{H}^{\text{CIM}} = \sum_{n=0}^{\infty} (E_0 + \varepsilon_n) \tilde{C}_n(t) C_n(t), \quad (3.3)$$

where $\{\varepsilon_n\}$ are the exact excitation energies,

$$\varepsilon_n \equiv E_n - E_0. \quad (3.4)$$

Equation (3.3) is clearly in diagonal normal-mode form, as expected. Because the eigenstates $|\Psi_n\rangle$ and $\langle \tilde{\Psi}_n|$ are separately normalized, we actually have $\tilde{C}_n = C_n^*$.

Let us denote generally by $\{\psi_n, \tilde{\psi}_n\} \equiv \{\psi_n(t), \tilde{\psi}_n(t)\}$ those amplitudes that diagonalize the effective Hamiltonian around a particular point in the phase space. In the CIM case we thus have the straightforward connection $\psi_n \equiv C_n$, $\tilde{\psi}_n \equiv \tilde{C}_n = C_n^*$; $n \geq 0$. We note that in the CIM the amplitudes $\{\psi_n(t), \tilde{\psi}_n(t)\}$ are simply the time-dependent expansion coefficients in the Schrödinger picture and should not be confused with the previous coordinate-space representations $\langle x | \Psi_n \rangle \equiv \psi_n(x)$ and $\langle \tilde{\Psi}_n | x \rangle \equiv \tilde{\psi}_n(x)$ of the Schrödinger energy eigenfunctions.

Furthermore, the temporal action functional $\mathcal{A}_0$ of Eq. (2.1) is trivially found to be given in the Bargmann-space representation of the CIM parametrization by

$$\mathcal{A}_0^{\text{CIM}} = i \int_{t_1}^{t_2} dt \sum_{n=0}^{\infty} \tilde{\psi}_n \dot{\psi}_n, \quad (3.5)$$

where $\dot{f} \equiv df/dt$ for an arbitrary function $f = f(t)$, as usual. In the Bargmann-space representation of the CIM we thus have that the full action functional $\mathcal{A} = \mathcal{A}^{\text{CIM}}[\psi_n, \tilde{\psi}_n]$ is bilinear even for large deviations from the ground state. The conditions $\partial \mathcal{A} / \partial \tilde{\psi}_n = 0$ and $\partial \mathcal{A} / \partial \psi_n = 0$ trivially lead, respectively, to the canonical equations

$$i\dot{\psi}_n = \partial \bar{H} / \partial \tilde{\psi}_n, \quad -i\dot{\tilde{\psi}}_n = \partial \bar{H} / \partial \psi_n, \quad n \geq 0, \quad (3.6)$$

for any temporal action in the canonical form of Eq. (3.5). For the CIM energy expectation value, $\bar{H} \rightarrow \bar{H}^{\text{CIM}}$, of Eq. (3.3), we immediately have that $\{\psi_n, \tilde{\psi}_n\}$ are respectively the positive- and negative-frequency normal-mode coordinates, as expected:

$$\psi_n(t) = e^{-iE_n t} \psi_n(0); \quad \tilde{\psi}_n(t) = e^{iE_n t} \tilde{\psi}_n(0). \quad (3.7)$$

The CIM dynamics is accordingly completely integrable, although in a phase space of countably infinite ($\aleph_0$) dimensionality. Indeed, the present CIM treatment is nothing but the conventional linear formalism of quantum mechanics, albeit unconventionally described from the point of view of a classical phase space.

We note that the conservation of the norm $\langle \tilde{\Psi}(t) | \Psi(t) \rangle$ allows us to eliminate the dynamical variables $\tilde{\psi}_0(t)$, $\psi_0(t)$ from Eqs. (3.5), (3.6), and to replace $N^2(t)$ by unity in Eq. (3.3), whence only the amplitudes with $n = 1, 2, \dots, \infty$ remain. This is accomplished by a redefinition of the phases,

$$\psi_n(t) \rightarrow \psi_n(t) e^{-iE_0 t}; \quad \tilde{\psi}_n(t) \rightarrow \tilde{\psi}_n(t) e^{+iE_0 t},$$

and it leads to an additional term in the temporal action $\mathcal{A}_0^{\text{CIM}}$. However, this is not a particularly useful simplification.

We turn next to the two CCM parametrizations, and first restrict ourselves to a general *infinitesimal* displacement away from the stationary ground state, such that the parameters $\{C_n, \tilde{C}_n\}$ for $n \geq 1$ in Eq. (3.1) are infinitesimal. We may now rather readily calculate the corresponding infinitesimal displacements of the CCM amplitudes away from their respective stationary values, namely $\{s^0(z), \tilde{s}^0(z)\}$ for the NCCM and $\{\sigma^0(z), \tilde{\sigma}^0(z)\}$ for the ECCM, in the same Bargmann Hilbert space. Using the relation $s(z; t) = \ln[f(z; t)/f(0; t)]$, and Eqs. (2.7), (2.9), and (2.6), one may easily check that accurate to first order in the small amplitudes, Eq. (3.1) implies the relations (where we denote $\psi_n = C_n/C_0$, $\tilde{\psi}_n = \tilde{C}_n/\tilde{C}_0$),

$$s(z; t) = s^0(z) + \sum_{n=1}^{\infty} \psi_n(t) s^{+n}(z), \quad (3.8a)$$

$$\tilde{s}(z; t) = \tilde{s}^0(z) + \sum_{n=1}^{\infty} [\psi_n(t) \tilde{s}^{+n}(z) + \tilde{\psi}_n(t) \tilde{s}^{-n}(z)], \quad (3.8b)$$

in which the various coefficients are defined as

$$s^{+n}(z) \equiv \frac{f^n(z)}{f^0(z)} - \frac{f^n(0)}{f^0(0)} = r_n(z) - r_n(0), \quad (3.9)$$

$$\tilde{s}^{+n}(z) \equiv \tilde{s}^{0n}(z), \quad \tilde{s}^{-n}(z) = \tilde{s}^{n0}(z).$$

We shall show below that this parametrization for the NCCM case indeed diagonalizes the effective action functional in agreement with the chosen notational convention. In Section IV we also prove that the parametrization is complete in the sense that all NCCM-representable states can be so parametrized.

We note from Eq. (2.11) that Eq. (3.8) implies that $\tilde{s}(0; t) = \tilde{s}^0(0) = 1$ for all t . By analogy with the relationship between $s(z)$ and $\hat{s}(x)$ in Eq. (2.13), it is convenient for later purposes to define a set of distributions $\{\hat{s}_n^+(x) | n = 1, 2, \dots\}$ relating to the

new functions $s^{+n}(z)$ which also enter Eq. (3.8) for $s(z; t)$ when it is perturbed away from its stationary value $s^0(z)$,

$$s^{+n}(z) \equiv \int_{-\infty}^{\infty} dx (e^{xz} - 1) \hat{s}_n^+(x), \quad \hat{s}_n^+(x) = \int_{-\infty}^{\infty} \frac{dy}{2\pi} e^{-iyx} \frac{f^n(iy)}{f^0(iy)}, \quad n \geq 1. \quad (3.10)$$

As emphasized in Section III of paper II, the integration contours in integrals of the above kind can in principle be chosen quite freely such that $x \in L'$ and $iy \in L$, where L and L' are a "conjugate" pair of lines; the restriction is that the zeros of the holomorphic wave functions must be avoided. We should keep this freedom in mind in all the integral expressions to come, although they are generically written using the real axis for L' and the imaginary axis for L .

By making use of Eq. (2.14) and the relation $\tilde{\sigma}(z; t) = \ln \tilde{s}(z; t)$, we may also derive the corresponding ECCM results accurate to first order in the amplitudes $\{\psi_n, \tilde{\psi}_n\}$. We find

$$\sigma(z; t) = \sigma^0(z) + \sum_{n=1}^{\infty} [\psi_n(t) \sigma^{+n}(z) + \tilde{\psi}_n(t) \sigma^{-n}(z)], \quad (3.11a)$$

$$\tilde{\sigma}(z; t) = \tilde{\sigma}^0(z) + \sum_{n=1}^{\infty} [\psi_n(t) \tilde{\sigma}^{+n}(z) + \tilde{\psi}_n(t) \tilde{\sigma}^{-n}(z)], \quad (3.11b)$$

where the various coefficients are defined as

$$\begin{aligned} \sigma^{+n}(z) &\equiv \int_{-\infty}^{\infty} dx (e^{xz} - 1) [\tilde{s}^{00}(x) \hat{s}_n^+(x) + \tilde{s}^{0n}(x) \hat{s}_0(x)], \\ \sigma^{-n}(z) &\equiv \int_{-\infty}^{\infty} dx (e^{xz} - 1) \tilde{s}^{n0}(x) \hat{s}_0(x), \\ \tilde{\sigma}^{+n}(z) &\equiv \frac{\tilde{s}^{0n}(z)}{\tilde{s}^{00}(z)} = \tilde{r}_{0n}(z); \quad \tilde{\sigma}^{-n}(z) \equiv \frac{\tilde{s}^{n0}(z)}{\tilde{s}^{00}(z)} = \tilde{r}_{n0}(z), \end{aligned} \quad (3.12)$$

and where the function $\hat{s}_0(x)$ corresponds to the ground-state function $s^0(z)$ as in Eq. (2.13). As the notation indicates, it will again be shown that this parametrization is complete and diagonal in the ECCM case.

The important point in Eqs. (3.11) is that the connection between the additively separable functions $\sigma(z)$, $\tilde{\sigma}(z)$, and the coordinates $\{\psi_n, \tilde{\psi}_n\}$, is *linear*.

It is clear from the above derivation that for both CCM methods the energy expectation value $\bar{H}$ contains no terms linear in the parameters $\{\psi_n, \tilde{\psi}_n\}$ when calculated with either of the parametrizations of Eqs. (3.8) and (3.11). What is less obvious is that in each case the effective quadratic Hamiltonian $\bar{H}_2$ (i.e., $\bar{H}$ curtailed at second-order-terms in $\{\delta s, \delta \tilde{s}\}$ and $\{\delta \sigma, \delta \tilde{\sigma}\}$, respectively) is actually diagonalized by these parametrizations, as we demonstrate explicitly below. Before

doing so, however, we first calculate the temporal action functional and show that it, too, is in canonical form for both parametrizations.

The NCCM form of the temporal action is trivially written using Eq. (2.2) in either of the forms,

$$\mathcal{A}_0^{\text{NCCM}} = i \int_{t_1}^{t_2} dt \tilde{s} \left(\frac{d}{dz}; t \right) \dot{s}(z; t) \Big|_{z=0} = i \int_{t_1}^{t_2} dt \dot{s} \left(\frac{d}{dz}; t \right) \tilde{s}(z; t) \Big|_{z=0}. \quad (3.13)$$

The first of these forms, together with definition (2.9) of the Fourier transform $\tilde{s}_F$, immediately yields the expression

$$\mathcal{A}_0^{\text{NCCM}} = i \int_{t_1}^{t_2} dt \int_{-\infty}^{\infty} \frac{dx}{2\pi} \tilde{s}_F(x; t) \dot{s}(ix; t). \quad (3.14a)$$

Similarly, use of definition (2.13) in the second form in Eq. (3.13) yields the alternative expression

$$\mathcal{A}_0^{\text{NCCM}} = i \int_{t_1}^{t_2} dt \int_{-\infty}^{\infty} dx \tilde{s}(x; t) \dot{\hat{s}}(x; t), \quad (3.14b)$$

where we have also made use of the explicit NCCM normalization, $\tilde{s}(0; t) = 1$ for all times t , in order to neglect the term involving a total time derivative, as usual. Finally, by adding to the integrand in Eq. (3.14b) the (irrelevant) total time derivative $(d/dt)(\tilde{\sigma}\hat{\sigma} - \tilde{s}\hat{s})$, and by making use of the definitions in Eqs. (2.8) and (2.14), we also have the equivalent ECCM form for the temporal action,

$$\mathcal{A}_0^{\text{ECCM}} = i \int_{t_1}^{t_2} dt \int_{-\infty}^{\infty} dx \tilde{\sigma}(x; t) \dot{\hat{\sigma}}(x; t). \quad (3.15)$$

By inserting the representation of Eq. (3.8) into Eq. (3.14a) and by making use of Eq. (2.10), we have

$$\begin{aligned} \mathcal{A}_0^{\text{NCCM}} = & i \int_{t_1}^{t_2} dt \int_{-\infty}^{\infty} \frac{dx}{2\pi} \left\{ \tilde{f}_F^0(x) f^0(ix) + \sum_{m=1}^{\infty} [\psi_m \tilde{f}_F^0(x) f^m(ix) + \tilde{\psi}_m \tilde{f}_F^m(x) f^0(ix)] \right\} \\ & \times \sum_{n=1}^{\infty} \dot{\psi}_n \left[\frac{f^n(ix)}{f^0(ix)} - \frac{f^n(0)}{f^0(0)} \right]. \end{aligned}$$

The normalization condition (2.5) then readily yields

$$\begin{aligned} \mathcal{A}_0^{\text{NCCM}} = & i \int_{t_1}^{t_2} dt \frac{d}{dt} \left[- \sum_{n=1}^{\infty} \frac{f^n(0)}{f^0(0)} \psi_n + \frac{1}{2} \sum_{m=1}^{\infty} \sum_{n=1}^{\infty} \psi_m \psi_n \right. \\ & \left. \times \int_{-\infty}^{\infty} \frac{dx}{2\pi} \frac{\tilde{f}_F^0(x) f^m(ix) f^n(ix)}{f^0(ix)} \right] + i \int_{t_1}^{t_2} dt \sum_{n=1}^{\infty} \tilde{\psi}_n \dot{\psi}_n. \end{aligned}$$

As usual, the term involving the total time derivative may be set to zero, to give the canonical form

$$\mathcal{A}_0^{\text{NCCM}} = i \int_{t_1}^{t_2} dt \sum_{n=1}^{\infty} \tilde{\psi}_n \dot{\psi}_n, \quad (3.16)$$

when $\{s(z; t), \tilde{s}(z; t)\}$ are parametrized as in Eq. (3.8).

Similarly, in the ECCM case we may insert Eq. (3.11) into Eq. (3.15) to obtain

$$\begin{aligned} \mathcal{A}_0^{\text{ECCM}} = & i \int_{t_1}^{t_2} dt \frac{d}{dt} \int_{-\infty}^{\infty} dx \left\{ \tilde{\sigma}^0(x) \sigma(x; t) + \frac{1}{2} \sum_{m=1}^{\infty} \sum_{n=1}^{\infty} \frac{\hat{s}_0(x)}{\tilde{s}^{00}(x)} \right. \\ & \times [\tilde{s}^{0m}(x) \psi_m + \tilde{s}^{m0}(x) \tilde{\psi}_m] [\tilde{s}^{0n}(x) \psi_n + \tilde{s}^{n0}(x) \tilde{\psi}_n] \Big\} \\ & + i \int_{t_1}^{t_2} dt \sum_{m=1}^{\infty} \sum_{n=1}^{\infty} \left\{ \psi_m \dot{\psi}_n \int_{-\infty}^{\infty} dx \tilde{s}^{0m}(x) \hat{s}_n^+(x) \right. \\ & \left. + \tilde{\psi}_m \dot{\tilde{\psi}}_n \int_{-\infty}^{\infty} dx \tilde{s}^{m0}(x) \hat{s}_n^+(x) \right\}. \end{aligned} \quad (3.17)$$

The first term in Eq. (3.17) again involves a total time derivative and may hence be set to zero. The remaining two integrals are readily evaluated by making use of Eqs. (2.9)–(2.10), together with the definition (3.10) and the normalization relation (2.5). We find

$$\int_{-\infty}^{\infty} dx \tilde{s}^{0m}(x) \hat{s}_n^+(x) = \int_{-\infty}^{\infty} \frac{dx}{2\pi} \frac{\tilde{f}_F^0(x) f^m(ix) f^n(ix)}{f^0(ix)}, \quad m \neq 0 \neq n, \quad (3.18a)$$

$$\int_{-\infty}^{\infty} dx \tilde{s}^{m0}(x) \hat{s}_n^+(x) = \delta_{m,n}, \quad m \neq 0 \neq n. \quad (3.18b)$$

By using the obvious symmetry in the indices m and n from the result of Eq. (3.18a), we may readily turn the first of the remaining integrals in Eq. (3.17) into a total time derivative. The remaining term is then evaluated from Eq. (3.18b) to show, finally, that $\mathcal{A}_0^{\text{ECCM}}$ also has the canonical form

$$\mathcal{A}_0^{\text{ECCM}} = i \int_{t_1}^{t_2} dt \sum_{n=1}^{\infty} \tilde{\psi}_n \dot{\psi}_n, \quad (3.19)$$

when $\{\sigma(z; t), \tilde{\sigma}(z; t)\}$ are parametrized as in Eq. (3.11).

We now return to the evaluation of the effective quadratic Hamiltonian and begin with the NCCM parametrization of Eq. (3.8) for a state perturbed away from the stationary ground state. The state is given in terms of a set of time-dependent perturbative parameters $\{\psi_m, \tilde{\psi}_m\}$, which we have initially taken to be infinitesimal.

A straightforward insertion of Eqs. (3.8) and (3.9) into the general expressions (2.15)–(2.16) gives for the energy expectation value in this NCCM parametrization,

$$\begin{aligned} \bar{H}^{\text{NCCM}} = & \int_{-\infty}^{\infty} \frac{dx}{2\pi} \tilde{f}_F^0(x) \left\{ 1 + \sum_{l=1}^{\infty} [\psi_l r_l(ix) + \tilde{\psi}_l \tilde{f}_F^l(x) / \tilde{f}_F^0(x)] \right\} \\ & \times \exp \left[- \sum_{m=1}^{\infty} \psi_m r_m(ix) \right] H \left(ix, -i \frac{d}{dx} \right) f_0(ix) \exp \left[\sum_{n=1}^{\infty} \psi_n r_n(ix) \right]. \end{aligned} \quad (3.20)$$

By expanding the two exponential terms in Eq. (3.20), it is a relatively simple matter to express $\bar{H}^{\text{NCCM}}$ in the form

$$\begin{aligned} \bar{H}^{\text{NCCM}} = & \sum_{n=0}^{\infty} \frac{1}{n!} \sum_{l_1=1}^{\infty} \cdots \sum_{l_n=1}^{\infty} \left[\langle | \bar{H} | l_1 \cdots l_n \rangle^{\text{NCCM}} \right. \\ & \left. + \sum_{k_1=1}^{\infty} \tilde{\psi}_{k_1} \langle k_1 | \bar{H} | l_1 \cdots l_n \rangle^{\text{NCCM}} \right] \psi_{l_1} \cdots \psi_{l_n}, \end{aligned} \quad (3.21)$$

where

$$\begin{aligned} \langle | \bar{H} | l_1 \cdots l_n \rangle^{\text{NCCM}} \equiv & \sum_{j=0}^n \frac{(-1)^{j+1} (j-1) n!}{j! (n-j)!} \int_{-\infty}^{\infty} \frac{dx}{2\pi} \tilde{f}_F^0(x) r_{l_1}(ix) \cdots r_{l_j}(ix) \\ & \times H \left(ix, -i \frac{d}{dx} \right) f^0(ix) r_{l_{j+1}}(ix) \cdots r_{l_n}(ix), \end{aligned} \quad (3.22a)$$

$$\begin{aligned} \langle k_1 | \bar{H} | l_1 \cdots l_n \rangle^{\text{NCCM}} \equiv & \sum_{j=0}^n \frac{(-1)^j n!}{j! (n-j)!} \int_{-\infty}^{\infty} \frac{dx}{2\pi} \tilde{f}_F^{k_1}(x) r_{l_1}(ix) \cdots r_{l_j}(ix) \\ & \times H \left(ix, -i \frac{d}{dx} \right) f^0(ix) r_{l_{j+1}}(ix) \cdots r_{l_n}(ix), \end{aligned} \quad (3.22b)$$

and where the functions $\{r_l(z)\}$ are defined in Eq. (2.6).

It is also clear that the matrix elements in Eq. (3.21) may be equivalently replaced by their symmetrized counterparts,

$$\begin{aligned} \langle | \bar{H} | l_1 \cdots l_n \rangle_S^{\text{NCCM}} & \equiv \frac{1}{n!} \sum_{\mathcal{P}\{l_j\}} \langle | \bar{H} | l_1 \cdots l_n \rangle^{\text{NCCM}}, \\ \langle k_1 | \bar{H} | l_1 \cdots l_n \rangle_S^{\text{NCCM}} & \equiv \frac{1}{n!} \sum_{\mathcal{P}\{l_j\}} \langle k_1 | \bar{H} | l_1 \cdots l_n \rangle^{\text{NCCM}}, \end{aligned} \quad (3.23)$$

in which the sums over $\mathcal{P}\{l_j\}$ run over all $n!$ permutations of the indices $(l_1, \dots, l_n)$.

With the above definitions, it is also clear that the matrix elements may formally be expressed as the following partial differentials evaluated at the stationary point,

$$\begin{aligned}\langle | \bar{H} | l_1 \dots l_n \rangle_S^{\text{NCCM}} &= \frac{\partial^n}{\partial \psi_{l_1} \dots \partial \psi_{l_n}} \bar{H}^{\text{NCCM}} \Big|_0, \\ \langle k_1 | \bar{H} | l_1 \dots l_n \rangle_S^{\text{NCCM}} &= \frac{\partial^{n+1}}{\partial \tilde{\psi}_{k_1} \partial \psi_{l_1} \dots \partial \psi_{l_n}} \bar{H}^{\text{NCCM}} \Big|_0,\end{aligned}\quad (3.24)$$

The matrix elements of the effective quadratic Hamiltonian $\bar{H}_2^{\text{NCCM}}$ may now be evaluated from the explicit expressions in Eq. (3.22). By making use of Eqs. (2.4)–(2.5), it is simple to show that

$$\begin{aligned}\langle | \bar{H} | \rangle^{\text{NCCM}} &= E_0, & \langle | \bar{H} | l \rangle^{\text{NCCM}} &= \langle l | \bar{H} | \rangle^{\text{NCCM}} = 0, \\ \langle | \bar{H} | lm \rangle^{\text{NCCM}} &= 0, & \langle k | \bar{H} | l \rangle^{\text{NCCM}} &= \varepsilon_l \delta_{k,l},\end{aligned}\quad (3.25)$$

and hence that the effective quadratic NCCM Hamiltonian which governs the dynamics of infinitesimal displacements away from the stationary ground state is diagonalized (i.e., put into normal modes) by the parametrization of Eq. (3.8),

$$\bar{H}_2^{\text{NCCM}} = E_0 + \sum_{n=1}^{\infty} \varepsilon_n \tilde{\psi}_n \psi_n. \quad (3.26)$$

We note that the CIM and NCCM expansions of Eqs. (3.4) and (3.26) respectively only agree for purposes of linear response, i.e., for infinitesimal perturbations away from the ground state. For the case of arbitrary finite perturbations away from equilibrium, we may continue to use the parametrization of Eqs. (3.8)–(3.9), but we can no longer truncate the expansion (3.21) of $\bar{H}^{\text{NCCM}}$ at the second-order level (i.e., at the $n=2$ term). In this general case the NCCM amplitudes $\{\psi_n, \tilde{\psi}_n\}$ clearly only agree with their CIM counterparts by the neglect of second- and higher-order terms. Once we have passed beyond treating the original CIM parameters $\{\psi_n, \tilde{\psi}_n\}$ in Eq. (3.1) as being infinitesimal, we should then indicate their counterparts in the NCCM expansions in Eq. (3.8) by a different symbol, or by the addition of an NCCM superscript or some such device. Nevertheless, we do *not* adopt any such explicit notation henceforth, in the belief that the careful reader, once forewarned, will not thereby be confused.

Whereas the CIM energy expectation value $\bar{H}^{\text{CIM}}$ is genuinely exactly quadratic in its normal-mode coordinates $\{\psi_n, \tilde{\psi}_n\}$, the same is not true in either the NCCM or the ECCM. Thus, both $\bar{H}^{\text{NCCM}}$ and $\bar{H}^{\text{ECCM}}$ are nonlinear expansions of their respective normal-mode coordinates $\{\psi_n, \tilde{\psi}_n\}$, which diagonalize the corresponding effective quadratic Hamiltonian in each case. In the NCCM case, $\bar{H}$ is still linear in the coordinates $\{\tilde{\psi}_n\}$ but not in the $\{\psi_n\}$, whereas in the ECCM case $\bar{H}$ is genuinely nonlinear in both sets of normal-mode coordinates.

In order to demonstrate this nonlinearity explicitly, we now calculate the two third-order terms, $\langle | \bar{H} | lmn \rangle^{\text{NCCM}}$ and $\langle k | \bar{H} | lm \rangle^{\text{NCCM}}$, in the expansion (3.21)

for $\bar{H}^{\text{NCCM}}$. In particular, we aim to show that they are finite, and hence are expressible in terms of convergent integrals. From Eq. (3.22a) we have

$$\begin{aligned} \langle | \bar{H} | lmn \rangle^{\text{NCCM}} = & \int_{-\infty}^{\infty} \frac{dx}{2\pi} \tilde{f}_F^0(x) \left[H \left(ix, -i \frac{d}{dx} \right) r_l(ix) r_m(ix) r_n(ix) \right. \\ & - 3r_l(ix) r_m(ix) H \left(ix, -i \frac{d}{dx} \right) r_n(ix) \\ & \left. + 2r_l(ix) r_m(ix) r_n(ix) H \left(ix, -i \frac{d}{dx} \right) \right] f_0(ix). \end{aligned}$$

By making use of Eqs. (2.4), we readily simplify the above expression,

$$\langle | \bar{H} | lmn \rangle^{\text{NCCM}} = 3(E_0 - E_n) \int_{-\infty}^{\infty} \frac{dx}{2\pi} \tilde{f}_F^0(x) f_0(ix) r_l(ix) r_m(ix) r_n(ix). \quad (3.27a)$$

From Eq. (3.22b) we similarly find

$$\begin{aligned} \langle k | \bar{H} | lm \rangle^{\text{NCCM}} = & \int_{-\infty}^{\infty} \frac{dx}{2\pi} \tilde{f}_F^k(x) \left[H \left(ix, -i \frac{d}{dx} \right) r_l(ix) r_m(ix) \right. \\ & - 2r_l(ix) H \left(ix, -i \frac{d}{dx} \right) r_m(ix) \\ & \left. + r_l(ix) r_m(ix) H \left(ix, -i \frac{d}{dx} \right) \right] f_0(ix), \end{aligned}$$

which may also be simplified to yield

$$\langle k | \bar{H} | lm \rangle^{\text{NCCM}} = (E_k - 2E_m + E_0) \int_{-\infty}^{\infty} \frac{dx}{2\pi} \tilde{f}_F^k(x) f_0(ix) r_l(ix) r_m(ix). \quad (3.27b)$$

Finally, Eqs. (3.27a), (3.27b) may also be written in the symmetrized forms,

$$\langle | \bar{H} | lmn \rangle_S^{\text{NCCM}} = -(\varepsilon_l + \varepsilon_m + \varepsilon_n) \int_{-\infty}^{\infty} \frac{dx}{2\pi} \tilde{s}_F^{00}(x) r_l(ix) r_m(ix) r_n(ix), \quad (3.28a)$$

$$\langle k | \bar{H} | lm \rangle_S^{\text{NCCM}} = (\varepsilon_k - \varepsilon_l - \varepsilon_m) \int_{-\infty}^{\infty} \frac{dx}{2\pi} \tilde{s}_F^{k0}(x) r_l(ix) r_m(ix). \quad (3.28b)$$

It is clear from the asymptotic behaviour of the functions $\tilde{s}_F^{mn}(x)$ and $r_l(ix)$ for large values of $|x|$, given by Eqs. (3.45) of II and (2.6), respectively, that the integrals in Eqs. (3.28a), (3.28b) are convergent. Indeed, it is similarly clear that *all* of the matrix elements involved in the expansion (3.21) for $\bar{H}^{\text{NCCM}}$, as given by Eqs. (3.22a), (3.22b), are finite and convergent expansions. We note, however, that the coefficients of fourth and higher orders cannot generally be simplified to the

extent of eliminating any explicit reference to the potential function U , as in the case of the third-order coefficients above.

We turn now to the comparable ECCM evaluation of the energy expectation value, $\bar{H}^{\text{ECCM}}$. That is, we now consider the parametrization of the state *arbitrarily* perturbed away from the ground state, given in terms of the ECCM functions $\{\sigma(z; t), \tilde{\sigma}(z; t)\}$ of Eq. (3.11). Nevertheless, as we have already seen in Section II, the average-value functional $\bar{H}$ is most readily evaluated in terms of the NCCM functions $\{s(z; t), \tilde{s}(z; t)\}$ as in Eq. (2.16). The corresponding NCCM function $\tilde{s}(z; t)$ is given immediately from Eqs. (2.8) and (3.11) as

$$\tilde{s}(z; t) = \tilde{s}^0(z) e^{Z(z; t)}, \quad (3.29)$$

$$Z(z; t) \equiv \sum_{n=1}^{\infty} [\psi_n(t) \tilde{\sigma}^{+n}(z) + \tilde{\psi}_n(t) \tilde{\sigma}^{-n}(z)]. \quad (3.30)$$

Similarly, the NCCM function $s(z; t)$, parametrized as in Eq. (2.13) in terms of the function $\hat{s}(x; t)$, is also readily given from Eqs. (3.11)–(3.12), and by comparison with Eq. (2.14), as

$$\hat{s}(x; t) = \hat{s}_0(x) [1 + Z(x; t)] e^{-Z(x; t)} + \sum_{n=1}^{\infty} \psi_n(t) \hat{s}_n^{+}(x) e^{-Z(x; t)}, \quad (3.31)$$

where we have made use of Eqs. (3.12) and (3.29).

We may now expand $\hat{s}(x; t)$ and $s(z; t)$ as

$$\begin{aligned} \hat{s}(x; t) &= \hat{s}_0(x) + \sum_{m=1}^{\infty} \hat{s}^{(m)}(x; t), \\ s(z; t) &= s^0(z) + \sum_{m=1}^{\infty} s^{(m)}(z; t) \equiv s^0(z) + \delta s(z; t), \end{aligned} \quad (3.32)$$

where, by definition, $f^{(m)}(z; t) \equiv [f(z; t)]^{(m)}$ is the m th-order piece of an (arbitrary) function $f(z; t)$ in terms of its expansion in powers of $\{\psi_n(t), \tilde{\psi}_n(t)\}$. For example, Eqs. (3.30)–(3.31) give the first-order term

$$\hat{s}^{(1)}(x; t) = \sum_{n=1}^{\infty} \psi_n(t) \hat{s}_n^{+}(x), \quad (3.33)$$

and hence, from Eqs. (2.13) and (3.10),

$$s^{(1)}(z; t) = \sum_{n=1}^{\infty} \psi_n(t) s^{+n}(z). \quad (3.34a)$$

From Eq. (3.9), we may also write Eq. (3.34a) as

$$\begin{aligned} s^{(1)}(z; t) &= \sum_{n=1}^{\infty} \psi_n(t) r_n(z) - \phi(t), \\ \phi(t) &\equiv \sum_{n=1}^{\infty} \psi_n(t) r_n(0). \end{aligned} \quad (3.34b)$$

We note in particular that since in Eq. (2.16) the function $s(z; t)$ appears in the two combinations, $\exp(\pm s)$, we may henceforth equivalently set $\phi(t) \rightarrow 0$ in our evaluation of $\bar{H}$ in the form

$$\begin{aligned} \bar{H} &= \sum_{l, m, n=0}^{\infty} \bar{H}_{lmn}, \\ \bar{H}_{lmn} &\equiv \int_{-\infty}^{\infty} \frac{dx}{2\pi} \tilde{s}_F^{(l)}(x) [e^{-s(ix)}]^{(m)} H\left(ix, -i \frac{d}{dx}\right) [e^{s(ix)}]^{(n)}. \end{aligned} \quad (3.35)$$

Thus, for example, in our ECCM parametrization of the arbitrarily perturbed state, we may write

$$\begin{aligned} [e^{s(ix)}]^{(1)} &= f^0(ix) \sum_{n=1}^{\infty} \psi_n r_n(ix), \\ [e^{-s(ix)}]^{(1)} &= -\frac{1}{f^0(ix)} \sum_{n=1}^{\infty} \psi_n r_n(ix). \end{aligned} \quad (3.36)$$

The definition of Eq. (3.35) also immediately yields, for example,

$$\bar{H}_{n00}^{\text{ECCM}} = E_0 \delta_{n,0}, \quad (3.37)$$

where we have made use of Eq. (2.4) and the fact that $\tilde{s}^{(n)}(0) = 0$, since $Z(0) = 0$ from Eqs. (2.11) and (3.12). Similarly, by making use of Eqs. (3.29)–(3.30) and Eqs. (2.4), it is simple to prove the relation

$$\bar{H}_{10n}^{\text{ECCM}} + \bar{H}_{01n}^{\text{ECCM}} = \sum_{k=1}^{\infty} \tilde{\psi}_k E_k \int_{-\infty}^{\infty} \frac{dx}{2\pi} \tilde{f}_F^k(x) f^0(ix) [e^{\delta s(ix)}]^{(n)}. \quad (3.38)$$

We are now ready to demonstrate that, just as in the previous NCCM case, the effective quadratic ECCM Hamiltonian, $\bar{H}_2^{\text{ECCM}}$, that governs the dynamics of *infinitesimal* perturbations away from the ground state, is also diagonalized by the ECCM parametrization of Eq. (3.11). We first write

$$\bar{H}_j^{\text{ECCM}} \equiv \sum_{k=0}^j \bar{H}_{(k)}^{\text{ECCM}}, \quad (3.39a)$$

$$\bar{H}_{(k)}^{\text{ECCM}} \equiv \sum_{l, m, n=0}^{\infty} \bar{H}_{lmn}^{\text{ECCM}} \delta_{l+m+n, k}. \quad (3.39b)$$

Equations (3.37)–(3.38), together with the orthogonality condition (2.5), immediately show that $\bar{H}^{\text{ECCM}}$ contains no terms linear in $\{\psi_n, \tilde{\psi}_n\}$, i.e., $\bar{H}_{(1)}^{\text{ECCM}} = 0$. Furthermore, the second-order term $\bar{H}_{(2)}^{\text{ECCM}}$ is now also readily evaluated. The six individual terms which contribute in this case from Eq. (3.39b) are calculated from the definition (3.35) and by making use of Eqs. (3.29)–(3.34), together with the two Schrödinger equation relations (3.33b)–(3.34) and the orthogonality relation (2.5). We find,

$$\bar{H}_{200}^{\text{ECCM}} = 0, \quad (3.40a)$$

$$\begin{aligned} \bar{H}_{020}^{\text{ECCM}} = E_0 \int_{-\infty}^{\infty} \frac{dx}{2\pi} \tilde{f}_F^0(x) f^0(ix) \\ \times \left[\frac{1}{2} \sum_{m=1}^{\infty} \sum_{n=1}^{\infty} \psi_m \psi_n r_m(ix) r_n(ix) - s^{(2)}(ix) \right], \end{aligned} \quad (3.40b)$$

$$\begin{aligned} \bar{H}_{002}^{\text{ECCM}} = E_0 \int_{-\infty}^{\infty} \frac{dx}{2\pi} \tilde{f}_F^0(x) f^0(ix) \\ \times \left[\frac{1}{2} \sum_{m=1}^{\infty} \sum_{n=1}^{\infty} \psi_m \psi_n r_m(ix) r_n(ix) + s^{(2)}(ix) \right], \end{aligned} \quad (3.40c)$$

$$\bar{H}_{101}^{\text{ECCM}} + \bar{H}_{011}^{\text{ECCM}} = \sum_{n=1}^{\infty} E_n \tilde{\psi}_n \psi_n, \quad (3.40d)$$

$$\begin{aligned} \bar{H}_{110}^{\text{ECCM}} = -E_0 \sum_{n=1}^{\infty} \tilde{\psi}_n \psi_n - E_0 \int_{-\infty}^{\infty} \frac{dx}{2\pi} \tilde{f}_F^0(x) f^0(ix) \\ \times \sum_{m=1}^{\infty} \sum_{n=1}^{\infty} \psi_m \psi_n r_m(ix) r_n(ix). \end{aligned} \quad (3.40e)$$

It is then trivial to show that

$$\bar{H}_2^{\text{ECCM}} = E_0 + \sum_{n=1}^{\infty} \varepsilon_n \tilde{\psi}_n \psi_n, \quad (3.41)$$

when the ECCM parametrization of Eq. (3.11) is employed. Equation (3.41) is the precise analogue of its NCCM counterpart of Eq. (3.26) in which the NCCM parametrization of Eq. (3.8) is employed.

By analogy with Eq. (3.21) we may thus write the full expansion of $\bar{H}^{\text{ECCM}}$ in the form

$$\begin{aligned} \bar{H}^{\text{ECCM}} = E_0 + \sum_{n=1}^{\infty} \varepsilon_n \tilde{\psi}_n \psi_n + \sum_{\substack{m=0 \\ (m+n \geq 3)}}^{\infty} \sum_{n=0}^{\infty} \frac{1}{m! n!} \sum_{k_1=1}^{\infty} \cdots \sum_{k_m=1}^{\infty} \sum_{l_1=1}^{\infty} \cdots \sum_{l_n=1}^{\infty} \\ \times \langle k_1 \cdots k_m | \bar{H} | l_1 \cdots l_n \rangle^{\text{ECCM}} \tilde{\psi}_{k_1} \cdots \tilde{\psi}_{k_m} \psi_{l_1} \cdots \psi_{l_n}. \end{aligned} \quad (3.42)$$

We note that in the cases $m=0$ and $n=0$ in Eq. (3.42) the ECCM matrix elements simply take the forms $\langle \bar{H} | l_1 \dots l_n \rangle^{\text{ECCM}}$ and $\langle k_1 \dots k_m | \bar{H} \rangle^{\text{ECCM}}$, respectively. Once again, the general matrix element in Eq. (3.42) may be replaced by its fully symmetrized counterpart,

$$\begin{aligned} \langle k_1 \dots k_m | \bar{H} | l_1 \dots l_n \rangle_S^{\text{ECCM}} &\equiv \frac{1}{m! n!} \sum_{\mathcal{P}\{k_i\}} \sum_{\mathcal{P}\{l_j\}} \langle k_1 \dots k_m | \bar{H} | l_1 \dots l_n \rangle^{\text{ECCM}} \\ &= \frac{\partial^{m+n}}{\partial \tilde{\psi}_{k_1} \dots \partial \tilde{\psi}_{k_m} \partial \psi_{l_1} \dots \partial \psi_{l_n}} \bar{H}^{\text{ECCM}} \Big|_0, \end{aligned} \quad (3.43)$$

where the symbols have the same meaning as in Eqs. (3.23)–(3.24).

In order to illustrate the above expansion, we again calculate explicitly below all of the third-order terms in Eq. (3.42). By methods completely analogous to the derivation of the second-order terms above, we find that the 10 individual terms which contribute to $\bar{H}_{(3)}^{\text{ECCM}}$ in Eq. (3.39b) may be written

$$\bar{H}_{300}^{\text{ECCM}} = 0, \quad (3.44a)$$

$$\begin{aligned} \bar{H}_{030}^{\text{ECCM}} + \bar{H}_{003}^{\text{ECCM}} &= 2E_0 \sum_{l=1}^{\infty} \psi_l \int_{-\infty}^{\infty} \frac{dx}{2\pi} \tilde{f}_F^0(x) f'_l(ix) s^{(2)}(ix) \\ &= 2E_0 \sum_{l=1}^{\infty} \psi_l \int_{-\infty}^{\infty} dx \tilde{s}^{0l}(x) \hat{s}^{(2)}(x), \end{aligned} \quad (3.44b)$$

$$\begin{aligned} \bar{H}_{210}^{\text{ECCM}} + \bar{H}_{201}^{\text{ECCM}} &= \sum_{l=1}^{\infty} \varepsilon_l \psi_l \int_{-\infty}^{\infty} \frac{dx}{2\pi} \tilde{s}_F^{(2)}(x) r_l(ix) \\ &= \sum_{l=1}^{\infty} \varepsilon_l \psi_l \int_{-\infty}^{\infty} dx \tilde{s}^{(2)}(x) \hat{s}_l^+(x), \end{aligned} \quad (3.44c)$$

$$\begin{aligned} \bar{H}_{120}^{\text{ECCM}} &= E_0 \int_{-\infty}^{\infty} \frac{dx}{2\pi} \sum_{n=1}^{\infty} [\psi_n \tilde{f}_F^0(x) f^n(ix) + \tilde{\psi}_n \tilde{f}_F^n(x) f^0(ix)] \\ &\quad \times \left[\frac{1}{2} \sum_{l=1}^{\infty} \sum_{m=1}^{\infty} \psi_l \psi_m r_l(ix) r_m(ix) - s^{(2)}(ix) \right], \end{aligned} \quad (3.44d)$$

$$\begin{aligned} \bar{H}_{102}^{\text{ECCM}} + \bar{H}_{012}^{\text{ECCM}} &= \sum_{n=1}^{\infty} E_n \tilde{\psi}_n \int_{-\infty}^{\infty} \frac{dx}{2\pi} \tilde{f}_F^n(x) f^0(ix) \\ &\quad \times \left[\frac{1}{2} \sum_{l=1}^{\infty} \sum_{m=1}^{\infty} \psi_l \psi_m r_l(ix) r_m(ix) + s^{(2)}(ix) \right], \end{aligned} \quad (3.44e)$$

$$\begin{aligned} \bar{H}_{021}^{\text{ECCM}} &= \sum_{n=1}^{\infty} E_n \psi_n \int_{-\infty}^{\infty} \frac{dx}{2\pi} \tilde{f}_F^0(x) f^n(ix) \\ &\quad \times \left[\frac{1}{2} \sum_{l=1}^{\infty} \sum_{m=1}^{\infty} \psi_l \psi_m r_l(ix) r_m(ix) - s^{(2)}(ix) \right], \end{aligned} \quad (3.44f)$$

$$\begin{aligned} \bar{H}_{111}^{\text{ECCM}} &= - \sum_{l=1}^{\infty} \sum_{m=1}^{\infty} \sum_{n=1}^{\infty} E_m \psi_l \psi_m \int_{-\infty}^{\infty} \frac{dx}{2\pi} r_l(ix) r_m(ix) \\ &\quad \times [\psi_n \tilde{f}_F^0(x) f^n(ix) + \tilde{\psi}_n \tilde{f}_F^n(x) f^0(ix)]. \end{aligned} \quad (3.44g)$$

It is thence a simple matter to show that

$$\begin{aligned} \bar{H}_{(3)}^{\text{ECCM}} &= \sum_{l=1}^{\infty} \varepsilon_l \psi_l \int_{-\infty}^{\infty} dx [\tilde{s}^{(2)}(x) \hat{s}_l^+(x) - \tilde{s}^{0l}(x) \hat{s}^{(2)}(x)] \\ &\quad + \sum_{n=1}^{\infty} \varepsilon_n \tilde{\psi}_n \int_{-\infty}^{\infty} dx \tilde{s}^{n0}(x) \hat{s}^{(2)}(x) \\ &\quad + \sum_{l=1}^{\infty} \sum_{m=1}^{\infty} \sum_{n=1}^{\infty} \left(\frac{1}{2} \varepsilon_n - \varepsilon_m \right) \psi_l \psi_m \psi_n \\ &\quad \times \int_{-\infty}^{\infty} \frac{dx}{2\pi} \tilde{f}_F^0(x) f^0(ix) r_l(ix) r_m(ix) r_n(ix) \\ &\quad + \sum_{l=1}^{\infty} \sum_{m=1}^{\infty} \sum_{n=1}^{\infty} \left(\frac{1}{2} \varepsilon_l - \varepsilon_m \right) \tilde{\psi}_l \psi_m \psi_n \\ &\quad \times \int_{-\infty}^{\infty} \frac{dx}{2\pi} \tilde{f}_F^l(x) f^0(ix) r_m(ix) r_n(ix). \end{aligned} \quad (3.45)$$

Finally, by making explicit use of Eqs. (3.29)–(3.31) to evaluate $\tilde{s}^{(2)}(x)$ and $\hat{s}^{(2)}(x)$, we find after some algebraic manipulations that $\bar{H}_{(3)}^{\text{ECCM}}$ may be expanded as

$$\begin{aligned} \bar{H}_{(3)}^{\text{ECCM}} &= \sum_{l,m,n=1}^{\infty} \left[\frac{1}{6} \langle lmn | \bar{H} | \rangle_S^{\text{ECCM}} \tilde{\psi}_l \tilde{\psi}_m \tilde{\psi}_n + \frac{1}{2} \langle lm | \bar{H} | n \rangle_S^{\text{ECCM}} \tilde{\psi}_l \tilde{\psi}_m \psi_n \right. \\ &\quad \left. + \frac{1}{2} \langle l | \bar{H} | mn \rangle_S^{\text{ECCM}} \tilde{\psi}_l \psi_m \psi_n + \frac{1}{6} \langle | \bar{H} | lmn \rangle_S^{\text{ECCM}} \psi_l \psi_m \psi_n \right], \end{aligned} \quad (3.46)$$

in terms of the four fully symmetrized third-order matrix elements,

$$\begin{aligned} \langle lmn | \bar{H} | \rangle_S^{\text{ECCM}} &= -(\varepsilon_l + \varepsilon_m + \varepsilon_n) \\ &\quad \times \int_{-\infty}^{\infty} dx \tilde{s}^{00}(x) \hat{s}_0(x) \tilde{\sigma}^{-l}(x) \tilde{\sigma}^{-m}(x) \tilde{\sigma}^{-n}(x), \end{aligned} \quad (3.47a)$$

$$\begin{aligned} \langle lm | \bar{H} | n \rangle_S^{\text{ECCM}} &= (\varepsilon_n - \varepsilon_l - \varepsilon_m) \\ &\quad \times \int_{-\infty}^{\infty} dx \tilde{s}^{00}(x) \tilde{\sigma}^{-l}(x) \tilde{\sigma}^{-m}(x) [\hat{s}_0(x) \tilde{\sigma}^{+n}(x) + \hat{s}_n^+(x)], \end{aligned} \quad (3.47b)$$

$$\begin{aligned}
\langle l | \bar{H} | mn \rangle_S^{\text{ECCM}} &= \langle l | \bar{H} | mn \rangle_S^{\text{NCCM}} + (\varepsilon_m + \varepsilon_n - \varepsilon_l) \\
&\times \int_{-\infty}^{\infty} dx \tilde{s}^{00}(x) \tilde{\sigma}^{-l}(x) [\hat{s}_0(x) \tilde{\sigma}^{+m}(x) \tilde{\sigma}^{+n}(x) \\
&+ \hat{s}_m^{+}(x) \tilde{\sigma}^{+n}(x) + \hat{s}_n^{+}(x) \tilde{\sigma}^{+m}(x)], \quad (3.47c)
\end{aligned}$$

$$\begin{aligned}
\langle | \bar{H} | lmn \rangle_S^{\text{ECCM}} &= \langle | \bar{H} | lmn \rangle_S^{\text{NCCM}} + (\varepsilon_l + \varepsilon_m + \varepsilon_n) \int_{-\infty}^{\infty} dx \tilde{s}^{00}(x) \\
&\times [\hat{s}_0(x) \tilde{\sigma}^{+l}(x) \tilde{\sigma}^{+m}(x) \tilde{\sigma}^{+n}(x) + \hat{s}_l^{+}(x) \tilde{\sigma}^{+m}(x) \tilde{\sigma}^{+n}(x) \\
&+ \hat{s}_m^{+}(x) \tilde{\sigma}^{+l}(x) \tilde{\sigma}^{+n}(x) + \hat{s}_n^{+}(x) \tilde{\sigma}^{+l}(x) \tilde{\sigma}^{+m}(x)]. \quad (3.47d)
\end{aligned}$$

We note that it is once again possible to show that all of the integrals in Eqs. (3.47a)–(3.47d) are convergent, by making use of the asymptotic properties for large values of $|x|$ of the functions $\tilde{s}^{mn}(x)$ and $\tilde{r}_{mn}(x)$, from Eqs. (3.49) of II and (2.12), respectively.

Although the final forms of both the NCCM and ECCM third-order matrix elements in their respective expansions of $\bar{H}$ are remarkably suggestive, higher-order matrix elements are considerably more complicated to determine. In particular, it is evident that the behaviour,

$$\langle k_1 \cdots k_m | \bar{H} | l_1 \cdots l_n \rangle_S \propto \left(\sum_{i=1}^m \varepsilon_{k_i} - \sum_{j=1}^n \varepsilon_{l_j} \right), \quad (3.48)$$

which is observed for all of the third-order elements in both the NCCM and ECCM, does not persist to higher orders. Nevertheless, it should be clear to the reader how to derive any desired higher-order coefficient, given either sufficient patience or a clever symbolic computer program.

Finally, we have explicitly demonstrated that both the NCCM parametrization of Eq. (3.8) and its ECCM counterpart of Eq. (3.11) manifestly diagonalize their respective energy expectation value functionals $\bar{H} = \bar{H}[\psi_n, \tilde{\psi}_n]$ at second-order level. The respective coordinates $\{\psi_n, \tilde{\psi}_n\}$ may thus be regarded as normal modes. We have also proven that the higher-order coefficients in each expansion are finite. Furthermore, as is characteristic of orthonormal expansions, it is evident that if a particular label n_j in the matrix element $\langle \cdots n_j \cdots | \bar{H} | \cdots \rangle$ or $\langle \cdots | \bar{H} | \cdots n_j \cdots \rangle$ becomes large, i.e., $n_j \rightarrow \infty$, the matrix element must vanish in this limit.

IV. CALCULATION OF THE NORMAL COORDINATES OF ARBITRARY STATES IN THE COUPLED-CLUSTER PHASE SPACES

In the previous section we have proven that the parametrizations of Eqs. (3.8) and (3.11) lead to properly diagonalized expansions around the ground state, and that for larger deviations the higher-order anharmonic matrix elements of the Hamiltonian can all be calculated in terms of convergent integral expressions.

Nevertheless, we have sidestepped the associated questions of completeness and CC-representability, which are concerned with what class of (otherwise arbitrary) Bargmann wave functions $\{f(z), \tilde{f}(z)\}$ can be represented via the parametrizations implied by either Eq. (3.8) or Eq. (3.11). Thus, in the NCCM case, for example, we would need to enquire: (i) whether the function spaces spanned by $\{s^0(z), r_n(z) \mid n=1, 2, \dots\}$ and $\{\tilde{s}^0(z), \tilde{s}^{\pm n}(z) \mid n=1, 2, \dots\}$ are large enough to allow an arbitrary pair of normed functions $f(z), \tilde{f}(z)$ to be represented in the forms $f(z) = \exp s(z)$ and $f(d/dz)\tilde{f}(z) = \tilde{s}(z)$, respectively, with $s(z)$ and $\tilde{s}(z)$ expanded as in Eq. (3.8), and (ii) if not, how may we describe or characterize the class of states in the Hilbert space $\mathcal{H}$ that is so CC-representable. Another important question concerns the convergence of the expansion for the expectation value of the Hamiltonian or other operators using the normal-mode coordinates for a state that is not infinitesimally close to the ground state.

We seek a partial answer to these questions by calculating the exact values for the CCM coordinates $\{\psi_n, \tilde{\psi}_n\}$ in a particular chart φ_i , corresponding to some choice of the line L , for arbitrary but CC-representable states in the Hilbert space (c.f., Section III of paper II). This not only proves the completeness of the parametrizations, but also offers useful criteria for the CC-representability. For the sake of simplicity of notation, however, we write the formulae as if L were the imaginary axis, as in the previous section.

Thus we assume a state of the general form (3.1) with arbitrary coefficients $\{C_n, \tilde{C}_n = C_n^*\}$, obeying the normalization condition (3.2). Let us first introduce in the case of the NCCM the finite difference functions $\Delta s(z) \equiv s(z) - s^0(z) = \ln[f(z)/f(0)] - \ln[f^0(z)/f^0(0)]$ and $\Delta \tilde{s}(z) \equiv \tilde{s}(z) - \tilde{s}^0(z) = \sum_m \sum_n (\tilde{C}_m C_n - \delta_{m,0} \delta_{n,0}) \tilde{s}^{mn}(z)$. From Eq. (3.8a) we obtain, by shifting terms and multiplying with $f^0(z)$,

$$\sum_{m=1}^{\infty} \psi_m f^m(z) = f^0(z) \Delta s(z) + f^0(z) \sum_{m=1}^{\infty} \left[\psi_m \frac{f^m(0)}{f^0(0)} \right]. \quad (4.1)$$

Both sides of this equation can be expanded in the complete basis $\{f^n \mid n=0, 1, \dots\}$. By letting $z = ix$, multiplying both sides by $\tilde{f}_F^n(x)$, integrating over x , and using the orthonormality of Eq. (2.5) we obtain

$$\psi_n = \int_{-\infty}^{\infty} \frac{dx}{2\pi} \tilde{s}_F^{n0}(x) \Delta s(ix). \quad (4.2)$$

If both functions are Fourier-transformed, we find the alternative expression

$$\psi_n = \int_{-\infty}^{\infty} dx \tilde{s}^{n0}(x) \Delta \hat{s}(x), \quad (4.3)$$

where $\Delta \hat{s}(x) \equiv \hat{s}(x) - \hat{s}_0(x)$; here $\hat{s}_0(x)$ corresponds to the ground-state $s^0(z)$ according to Eq. (2.13).

We now verify that the component along f^0 in Eq. (4.1) vanishes. For that purpose we note that due to the completeness of the basis we have the relation

$$\sum_{n=0}^{\infty} \tilde{f}_{\text{F}}^n(x) f^n(iy) = 2\pi \delta(x-y). \quad (4.4)$$

By using this equation, together with Eqs. (4.2) and (2.10), we readily find

$$\begin{aligned} \sum_{n=1}^{\infty} \psi_n \frac{f^n(0)}{f^0(0)} &= \int_{-\infty}^{\infty} \frac{dx}{2\pi} \sum_{n=1}^{\infty} \frac{f^n(0)}{f^0(0)} \tilde{f}_{\text{F}}^n(x) f^0(ix) \Delta s(ix) \\ &= \Delta s(0) - \int_{-\infty}^{\infty} \frac{dx}{2\pi} \tilde{s}_{\text{F}}^{00}(x) \Delta s(ix). \end{aligned}$$

Noting that $\Delta s(0) = 0$, we may insert this result into the right-hand side of Eq. (4.1), multiply by $\tilde{f}_{\text{F}}^0(x)$, and integrate over x (while $z = ix$), and confirm that the terms in the right-hand side cancel, thus proving that its component along f^0 vanishes. This completes the proof that Eqs. (4.2)–(4.3) provide the correct and full solution to Eq. (3.8a) for arbitrary states.

To solve for the coefficients $\tilde{\psi}_n$ we take the Fourier transform of Eq. (3.8b), shift terms, divide by f^0 , and find

$$\sum_{m=1}^{\infty} \tilde{\psi}_m \tilde{f}_{\text{F}}^m(x) = \frac{\Delta \tilde{s}_{\text{F}}(x)}{f^0(ix)} - \frac{\tilde{f}_{\text{F}}^0(x)}{f^0(ix)} \sum_{m=1}^{\infty} \psi_m f^m(ix). \quad (4.5)$$

We substitute Eq. (4.2) into the right-hand side, apply the completeness relation of Eq. (4.4), and obtain

$$\sum_{m=1}^{\infty} \tilde{\psi}_m \tilde{f}_{\text{F}}^m(x) = \frac{\Delta \tilde{s}_{\text{F}}(x)}{f^0(ix)} - \tilde{f}_{\text{F}}^0(x) \left[\Delta s(ix) - \int_{-\infty}^{\infty} \frac{dy}{2\pi} \tilde{s}_{\text{F}}^{00}(y) \Delta s(iy) \right]. \quad (4.6)$$

Clearly both sides are orthogonal to the state f^0 . The component along f^n can be obtained by multiplying with $f^n(ix)$ and integrating; thus we obtain finally

$$\tilde{\psi}_n = \int_{-\infty}^{\infty} \frac{dx}{2\pi} \left[\Delta \tilde{s}_{\text{F}}(x) \frac{f^n(ix)}{f^0(ix)} - \tilde{s}_{\text{F}}^{0n}(x) \Delta s(ix) \right]. \quad (4.7)$$

Expressed through Fourier transforms in both terms we find the alternative form

$$\tilde{\psi}_n = \int_{-\infty}^{\infty} dx [\tilde{s}_n^+(x) \Delta \tilde{s}(x) - \tilde{s}^{0n}(x) \Delta \tilde{s}(x)]. \quad (4.8)$$

Equations (4.2)–(4.3) and (4.7)–(4.8) provide the complete solutions for the NCCM coefficients $\{\psi_n, \tilde{\psi}_n\}$ in terms of the coefficients $\{C_n, \tilde{C}_n = C_n^*\}$ that implicitly determine the difference functions Δs , $\Delta \tilde{s}$, $\Delta \tilde{s}$, and $\Delta \tilde{s}_{\text{F}}$.

The corresponding solutions are also easily found for the ECCM case. By using the representations of Eqs. (2.14) for $\Delta\sigma(z)$ in terms of $\Delta\hat{\sigma}(x)$ and (3.12) we can rewrite Eqs. (3.11) as

$$\begin{aligned}\Delta\hat{\sigma}(x) = & \sum_{m=1}^{\infty} \psi_m [\tilde{s}^{00}(x) \hat{s}_m^+(x) + \tilde{s}^{0m}(x) \hat{s}_0(x)] \\ & + \sum_{m=1}^{\infty} \tilde{\psi}_m \tilde{s}^{m0}(x) \hat{s}_0(x) + A\delta(x),\end{aligned}\quad (4.9a)$$

$$\tilde{s}^{00}(x) \Delta\tilde{\sigma}(x) = \sum_{m=1}^{\infty} \psi_m \tilde{s}^{0m}(x) + \sum_{m=1}^{\infty} \tilde{\psi}_m \tilde{s}^{m0}(x). \quad (4.9b)$$

Here A is an unspecified constant, which is allowed by the fact that the factor $(\exp xz - 1)$ in Eq. (3.12) is zero at $x=0$. Combining these equations we easily derive

$$\sum_{m=1}^{\infty} \psi_m \hat{s}_m^+(x) = \frac{\Delta\hat{\sigma}(x)}{\tilde{s}^{00}(x)} - \hat{s}_0(x) \Delta\tilde{\sigma}(x) - A\delta(x). \quad (4.10)$$

By taking the Fourier transform of both sides, multiplying with $\tilde{f}_F^n(x) f^0(ix)$ and integrating, we finally find the result

$$\psi_n = \int_{-\infty}^{\infty} dx \tilde{s}^{n0}(x) \left[\frac{\Delta\hat{\sigma}(x)}{\tilde{s}^{00}(x)} - \hat{s}_0(x) \Delta\tilde{\sigma}(x) \right]. \quad (4.11)$$

For the index $n=0$ we obtain a further consistency requirement, which fixes the value of A as

$$A = \int_{-\infty}^{\infty} dx [\Delta\hat{\sigma}(x) - \hat{\sigma}_0(x) \Delta\tilde{\sigma}(x)],$$

but which does not affect any of the ψ_n for $n \geq 0$.

From Eq. (4.9b) we obtain, by Fourier-transforming and shifting terms,

$$\sum_{m=1}^{\infty} \tilde{\psi}_m \tilde{f}_F^m(y) f^0(iy) = \int_{-\infty}^{\infty} dx e^{-ixy} \tilde{s}^{00}(x) \Delta\tilde{\sigma}(x) - \tilde{f}_F^0(y) \sum_{m=1}^{\infty} \psi_m f^m(iy). \quad (4.12)$$

We insert the result (4.11) into the right-hand side and use the easily proved intermediate result

$$\sum_{m=1}^{\infty} f^m(iy) \tilde{s}^{m0}(x) = e^{iyx} - f^0(iy) \tilde{s}^{00}(x), \quad (4.13)$$

and go on to multiply Eq. (4.12) by $f^n(iy)/f^0(iy)$ and integrate over y . After simplification we finally obtain

$$\begin{aligned} \tilde{\psi}_n = & \int_{-\infty}^{\infty} dx \Delta\tilde{\sigma}(x) [\tilde{s}^{00}(x) \hat{s}_n^+(x) + \tilde{s}^{0n}(x) \hat{s}_0(x)] \\ & - \int_{-\infty}^{\infty} dx \Delta\hat{\sigma}(x) \tilde{\sigma}^{+n}(x). \end{aligned} \quad (4.14)$$

It is also easily checked that for the index $n=0$ there is no additional problem. Equations (4.11) and (4.14) thus form the complete solution for the ECCM amplitudes.

In Appendix B of II we proved that the coupled-cluster coordinates $\{s_n, \tilde{s}_n, \tilde{\sigma}_n\}$ are all independent of the choice of the integration contour L out of which the function $s(z)$ is analytically continued. On the other hand, the amplitudes $\{\sigma_n\}$ were shown to depend on this choice but only to the extent of how L divides the zeros of $f(z)$ into two groups. To prove that also the NCCM or ECCM normal mode amplitudes $\{\psi_n, \tilde{\psi}_n\}$ are similarly dependent on L only in so far as the specific way it divides the zeros $\{z_m\}$ of $f(z)$ into two classes, we should go through the numerous equations in Sections III–IV and reformulate them using the general pair of lines L, L' . For example, the orthogonality relations of Eqs. (2.5) and the completeness relations (4.4) and (4.13) can be immediately thus generalized. This is instrumental in showing that the expressions for the exact NCCM or ECCM amplitudes $\{\psi_n, \tilde{\psi}_n\}$ as given in Eqs. (4.2)–(4.3) and (4.7) for the NCCM, and Eqs. (4.11) and (4.14) for the ECCM, respectively, are independent of the exact position of L and that they, instead, depend only on the discrete set of different ways to divide the zeros. As a side remark we note that, although the basic NCCM coupled-cluster amplitudes $\{s_n\}$ are in principle independent of the choice of L , the same is not true for the NCCM normal coordinates $\{\psi_n, \tilde{\psi}_n\}$. These *do* depend on how L divides the zeros.

We have proven in this section that the CCM normal-mode coordinates can be found even for states that are not close to the expansion point (say p_0), i.e., the ground state. However, this does not yet guarantee that the expansions in terms of these coordinates at an arbitrary point p for the average values of the Hamiltonian or other operators automatically converge. For our purpose it would be enough to know that they are asymptotic expansions in the sense that the low order terms are able to determine the differential geometry in an infinitesimal neighbourhood of the expansion point, for which purpose only the terms up to a finite order in the amplitudes $\psi_n, \tilde{\psi}_n$ will be needed. However, this is rather obvious if one considers the form of, e.g., the ECCM generating functional for the average values (and see Section IV in paper II). This is an expansion from which only a finite number of terms is needed for any usual polynomial operator, and the problem to consider is whether the expansion in powers of λ is asymptotic if the difference functions $\Delta\tilde{\sigma}(x)$, $\Delta\hat{\sigma}(x)$ are substituted by $\lambda \Delta\tilde{\sigma}(x)$, $\lambda \Delta\hat{\sigma}(x)$. We shall not, however, go into more detail here.

Let us finally briefly examine the conditions under which an arbitrary state $|\Psi\rangle$ of the Hilbert space $\mathcal{H}$ is CC-representable and under what circumstances it is possible to apply the results of the present section. The precise formulation of the necessary requirements is a nontrivial problem in functional analysis, and we will be satisfied with only a short remark.

A broad characterization of the CC-representable wave functions $\psi(x)$ is the property that they are smooth and very strongly confined. All of the above formalism easily goes through if we assume, for example, that the Schrödinger wave function $\psi(x)$ is a superposition of a *finite* number of eigenfunctions of the anharmonic oscillator. The asymptotic distribution of zeros of such a linear superposition is qualitatively identical to that of individual eigenstates, and the computations can be repeated step by step. Furthermore, this is sufficient because every normed wave function $\psi(x)$ can be arbitrarily well approximated, in the sense of the norm in $L^2([-\infty, \infty], \mathbb{C})$, by a finite number of basis functions. The argument also shows that the CC-representable states are dense in the Hilbert space.

V. ON THE GEOMETRICAL STRUCTURE OF THE COUPLED-CLUSTER PHASE SPACES

V.1. General Features

Each independent-cluster parametrization maps a pair $(\langle\tilde{\Psi}|, |\Psi\rangle)$ into a point p in an ICM phase space, which is a symplectic manifold. We can write formally

$$\begin{aligned} \text{CIM: } \mathcal{H}^* \times \mathcal{H} &\rightarrow \Gamma^{\text{CIM}}, \\ \text{NCCM: } \mathcal{H}^* \times \mathcal{H}/GL(1, \mathbb{C}) &\rightarrow \Gamma^{\text{NCCM}}, \\ \text{ECCM: } \mathcal{H}^* \times \mathcal{H}/GL(1, \mathbb{C}) &\rightarrow \Gamma^{\text{ECCM}}, \end{aligned} \quad (5.1)$$

where $\mathcal{H}^*$ is the dual space of the Hilbert space $\mathcal{H}$. In NCCM and ECCM the mapping is projective because of the intrinsic normalization requirements. The CIM map can in fact be understood as the identity. We shall speak about the original “from” spaces of these maps as the “state spaces.”

Due to the mutual independence of the bra and ket parametrizations the ICM phase spaces are “too large,” and the normalization condition of Eq. (3.2) together with the Hermiticity requirement, $\langle\tilde{\Psi}| = (|\Psi\rangle)^\dagger$, restrict the physical states to lie in only a part of the phase spaces, namely the submanifolds $\Gamma_{\text{phys}}^{\text{CIM}}$, $\Gamma_{\text{phys}}^{\text{NCCM}}$, and $\Gamma_{\text{phys}}^{\text{ECCM}}$, respectively. It is obvious that the phase spaces are locally differentiable manifolds, but in the CCM cases their topology is far from trivial for several reasons to be briefly discussed below. The most important complicating feature in the present case is the infinite dimensionality of the phase spaces, which must be taken carefully into account.

In the previous section we constructed the chart K_{p_0} , which is the normal coordinate system at the ground state p_0 of an ICM phase space. This coordinate system

was also shown to be able to describe a larger region around p_0 . We may similarly denote by K_p any coordinate system which is normal at some other point p , in the sense that the second-order Hamiltonian around p is diagonalized. In the coupled-cluster cases we may write $K_{p'}$ for the possible different diagonalized charts at the different points p' corresponding to the same physical state. These correspond to the different inequivalent integration contours L of Section III of paper II (and see also Section II) that were introduced to parametrize the function $s(z)$. We may also denote by K' the class of all charts determined by a line L , without requiring diagonality at any specific point p . Each particular choice to divide up the zeros provides a chart of some part of the phase space in terms of complex canonical coordinates. The union of all such charts for all CC-representable states is an atlas of the whole phase space.

It is also the case (and see Section IV) that the actual values of the CCM coordinates of a given state, e.g., $q = \{\psi_n, \tilde{\psi}_n\}$, in the chart $K_{p'}$ do not depend on the precise position of the line L as long as it divides the zeros z_m of $f(z)$ into two groups in the same given way. Only if L is moved across some zero, whence also the branch cut of $s(z)$ is swept to the other side of L , does a sudden change occur in the coordinates $\{\psi_n, \tilde{\psi}_n\}$, due to the necessity to jump to another chart. Thus the same physical state can in principle be described by a discrete number of different image points q' ($r = 1, 2, \dots$) in the CCM phase space.

As a matter of fact, it is easily shown that the various charts (or classes K' of them) covering a particular physical point are joined to each other smoothly through some continuous path in the phase space. To see this, let us consider two charts that correspond to divisions L and L_1 which differ only to the extent that one particular zero z_m lies between them. We construct the function

$$f(z; z_m, w) = f(z) \frac{1 - z/w}{1 - z/z_m} \quad (5.2)$$

from $f(z)$ by shifting the zero z_m to a new position w . The zero w can be transported around the line L through infinity and returned back from the other side to its original position z_m , pushing the line L to the displaced position L_1 . During the transformation the asymptotic properties of the holomorphic function $f(z; z_m, w)$ remain essentially unaffected, assuming that the state $f(z)$ is CC-representable, and in particular the saddle points of such integral formulae that determine the asymptotic properties of the functions $\phi(z) \equiv \exp(\frac{1}{2} z^2) f(z)$, $\chi(z) \equiv \exp(\frac{1}{2} z^2) f_F(z)$, and $\tilde{s}(z)$ remain qualitatively the same. The reason is that the infinite set of distant zeros with asymptotically increasing linear density have a dominating effect on the asymptotic properties of $f(z)$. Therefore the representative point $p(w)$ in the phase space Γ^{CCM} moves continuously. Because all the divisions of zeros that L creates can be reached from each other by a number of such steps, the various charts covering the neighbourhood of an arbitrary state are thus smoothly connected. This means that the CCM phase space is connected. However, it need not be simply connected.

Now let a state $|\Psi\rangle = (\langle\tilde{\Psi}|)^+$ change in a continuous fashion along some smooth path in the Hilbert space $\mathcal{H}$, $|\Psi\rangle = |\Psi(s)\rangle$, $s \geq 0$, where $|\Psi(0)\rangle$ is, for example, the ground state. The zeros $\{z_m(s)\}$ of the corresponding Bargmann wave function $f(z)$ then move smoothly in the complex plane. By displacing the integration route L in the z -plane so as to prevent any of the zeros from crossing it, the point $p(s) = \{\psi_n(s), \tilde{\psi}_n(s)\}$ in the CCM phase space also moves in a continuous way. However, it may in principle occasionally happen that the integration route becomes pinched between the zeros in such a way that a continuous deformation is no longer possible. Depending on the case, this may either indicate that the chart in question is not suitable for the particular region and should be replaced by another, or it might signify some intrinsic singularity in the CCM phase space such as, for example, the approach to a state which is not CC-representable.

The CCM map also displays the phenomenon of geometric phase or holonomy (or, more precisely, anholonomy, as Berry emphasizes [22]). If there are zeros on both sides of the contour L , it is obvious that closed continuous loops can be found in the state space such that some of the zeros of the corresponding holomorphic wave function $f(z)$ flow across L . An example of this kind was provided by Eq. (5.2), where a zero was transported via infinity; this did not actually demand zeros to be on both sides of L . Another way to accomplish the change is to map the set of zeros onto itself in a smooth way such that $z_m(s=0) = z_m$; $z_m(s=1) = z_{m-1}$, once a particular ordering of the zeros has been chosen. During the change the wave function may actually be the ground state of some adiabatically changing Hamiltonian. In this case the state typically remains CC-representable. It may be possible to prevent the zeros from crossing the line L which parametrizes the charts of class K' by moving L out of their way. In the end L will be displaced from its original position, whence the chart has changed smoothly to some member of another class K^* . The anholonomy in the NCCM or ECCM map given by Eq. (5.1) is discrete, by contrast with the more usual continuous case.

The zeros of the Bargmann wave function have recently received attention in the theory of chaotic systems. In Ref. [23] it was observed that classically integrable or otherwise regular systems lead, on quantization, to linear or quasilinear sets of regularly spaced zeros, whereas the quantized versions of classically chaotic systems seem to yield genuinely two-dimensional, widely spread arrays of zeros. Our present example of the anharmonic oscillator is in accordance with this trend. Since the distribution of zeros is connected to the geometric structure of the CCM phase spaces, it may be expected that the CCM manifolds of simple chaotic systems may be even (much) more complicated than in the present case.

Many of the rather pronounced complexities in the present case derive from the fact that a zero-dimensional ($d=0$) system does not have any properties of spatial locality. The concepts of "size extensivity" or "additive separability," which are central to the rationale for coupled cluster theory, are therefore meaningless; and the connected and disconnected diagrams give contributions which are of the same order of magnitude. In a sense the present CCM phase space resembles an

“internal” space (or fibre) of a more realistic field theory defined for higher spatial dimensionality $d > 0$.

The holomorphic formalism of the ECCM has been extended to the most general field-theoretic case in Ref. [18], allowing also for the anticommuting fermionic degrees of freedom. However, the representation remains formal so long as its basic assumptions have not been proven. Similarly, as soon as more than one degree of freedom is considered we are led to functions $F(z_1, \dots, z_n)$ of several complex variables, or, even worse, to functionals $F[z(x)]$ of fields $z(x)$ over some d -dimensional manifold M^d . For such cases there exist no simple factorization theorems analogous to the Weierstrass–Hadamard theorem. For example, the zeros of $F(z_1, \dots, z_n)$ are manifolds of $2n - 2$ real dimensions, and to our knowledge very little is known in general about their structure and distribution. Representations like those in Eqs. (2.13)–(2.14), which are crucial to the present formalism, have not been proven for such cases.

V.2. Metric Properties

We now try to analyse the structures of the CCM phase spaces quantitatively by using the standard methods of the theory of manifolds. Our main purpose is to analyze to what extent the formal nonlinearity of the coupled-cluster representation is a genuine property of the manifold. Since the CIM and NCCM are simplifications in comparison with the ECCM, we restrict ourselves to the latter case. There is no unique way to assign geometric or metric properties to a general manifold with a complicated overall structure. Here we choose to base our consideration on the charts K_p which locally diagonalise the Hamiltonian.

Because the ECCM Hamiltonian, Eq. (3.42), is nonlinear, a chart K_p which is diagonal at point p , is in general not diagonal at a neighbouring point p' . We wish to introduce the concepts of metric tensor and parallel transport in such a way that they are as fully compatible with the basic symplectic structure as possible. Therefore it is, for example, not readily possible to apply the theory of complex manifolds [24] in our case, although the coordinates $\{\psi_n, \tilde{\psi}_n\}$ are complex-valued. The problems are that the $\tilde{\psi}_n$ are not complex conjugates of ψ_n and that the transition functions (canonical transformations) between different diagonalizing charts K_p and $K_{p'}$ are not holomorphic functions of the coordinates, unless the dimensionality of the manifold is doubled by explicitly introducing the complex conjugate coordinates $\{\psi_n^*, \tilde{\psi}_n^*\}$. Only the CIM phase space admits a complex structure in a trivial way; it is a Kähler manifold.

We mention in passing that alternative metrisations for symplectic spaces have been introduced. Giraud and Rowe [25], for example, studied the collective submanifolds of a Hilbert space pertinent to the generator coordinate method. The submanifolds were orbits of certain collective Lie groups, such as the set of Glauber coherent states and the set of Slater determinants. As a matter of fact, both these examples are described in the ECCM as the manifolds of the lowest-order non-trivial truncations, namely the bosonic and the fermionic SUB 1 approximations. If one considers the underlying Hilbert space to be the flat complex Euclidean space

(as also in the present article, see below), the induced metric in the collective submanifolds makes them intrinsically curved. In contrast to [25], we now consider the complete CCM phase space which covers the whole of the state space. Use of the metric induced from the underlying Hilbert space would harmfully interfere with the linked-cluster nature of the CCM amplitudes. More precisely, the small displacements at a point p that diagonalise the metric induced from the Hilbert space would be not only quite different from the normal coordinates of K_p but (although we do not wish to expand on this point in the present article) also basically unlinked in terms of diagrammatic interpretation. Therefore we think that the metrisation suggested in [25] is not suitable for the CCM manifolds, although it is precisely the same as in our CIM case. Instead, we proceed differently.

We adopt the convention that all degrees of freedom (or coordinate directions) are treated equally and are considered to belong to the base space, which leaves no nontrivial "hair" to the fibre in the sense of the theory of fibre bundles. Our total space is then a tangent bundle, at least locally. To be consistent with standard notation, let us denote the coordinates of some chart by $\{x^\mu\} \equiv \{\psi_n, \tilde{\psi}_n\}$. We also denote $\psi_{\tilde{n}} \equiv \tilde{\psi}_n$, and use the notation $\tilde{n} = \tilde{n}$, $\tilde{\tilde{n}} = n$. The index $\bar{\mu}$ therefore denotes either $\tilde{n}$ or n depending on whether μ is n or $\tilde{n}$. We can imagine the differential coordinate "vector" dx^μ to be given in a block matrix form (with the convention that matrix indices are subscripts)

$$[dx]_\mu = \begin{bmatrix} d\psi_n \\ d\psi_{\tilde{n}} \end{bmatrix}, \quad (5.3)$$

where the square brackets are used to denote matrix representations. The tangent space $T_p M$ at each point p is a linear (infinite-dimensional) vector space, where the coordinate basis is defined by the vectors $e_\mu = \partial/\partial x^\mu$. The cotangent space $T_p^* M$ is spanned by the dual basis of one-forms dx^μ . We use dx^μ in the meaning of a small distance, whence it can be considered as the component of a vector.

The second-order Hamiltonian matrix at a point p is defined as

$$[H]_{\mu\nu} \equiv H_{\mu\nu} \equiv \frac{\partial^2 \bar{H}}{\partial x^\mu \partial x^\nu} \Leftrightarrow H = \begin{bmatrix} F & E^\top \\ E & \tilde{F} \end{bmatrix}, \quad (5.4)$$

where the block matrix consists of the submatrices E , F , and $\tilde{F}$ with matrix elements,

$$F_{mn} = \frac{\partial^2 \bar{H}}{\partial \psi_m \partial \psi_n}, \quad E_{\tilde{m}n} = \frac{\partial^2 \bar{H}}{\partial \psi_{\tilde{m}} \partial \psi_n} = E_{n\tilde{m}}^\top, \quad \tilde{F}_{\tilde{m}\tilde{n}} = \frac{\partial^2 \bar{H}}{\partial \psi_{\tilde{m}} \partial \psi_{\tilde{n}}}. \quad (5.5)$$

Clearly H is symmetric, $H = H^\top$. It is not, however, generally diagonal in the sense of Eq. (3.41). However, by performing a canonical transformation on the coordinates x^μ (or on the column vectors e_μ) the matrix H can be diagonalized. We denote the basis vectors that diagonalize H in $T_p M$ as $\hat{e}_\alpha \equiv e_\alpha^\mu e_\mu$ where the Einstein summation convention is employed for indices repeated once as a subscript

and once as a superscript; and the corresponding coordinates are denoted as $\hat{x}^z$. The difference vector dx may then be represented as $dx = e_\mu dx^\mu = \hat{e}_z d\hat{x}^z$; where $\{d\hat{x}^z\} = \{d\hat{x}^a, d\hat{x}^{\bar{a}}\}$ as before. The condition for the new basis is hence that

$$\bar{H}_{(2)}(x + dx) = \frac{1}{2} \sum_{\mu, \nu} H_{\mu\nu} dx^\mu dx^\nu = \frac{1}{2} \sum_{z, \beta} \hat{H}_{z\beta} d\hat{x}^z d\hat{x}^\beta \equiv \sum_a \varepsilon_a d\hat{x}^{\bar{a}} d\hat{x}^a. \quad (5.6)$$

The matrix $\hat{H}$ clearly has the form

$$\hat{H} = \begin{bmatrix} 0 & \varepsilon \\ \varepsilon & 0 \end{bmatrix}, \quad (5.7)$$

where ε is the diagonal submatrix with the entries appearing in Eq. (5.6), $[\varepsilon]_{ab} = \varepsilon_a \delta_{a, \bar{b}}$.

Since the diagonalizing basis plays a special role with regard to the Hamiltonian and its normal coordinates at the point p , we now let it define a non-coordinate basis in terms of which a (pseudo-)Riemannian metric may be introduced. We thus interpret the coefficients e_x^μ as vielbeins. By defining the matrix A and its inverse A^{-1} as

$$[A]_{\mu x} \equiv e_x^\mu \equiv \frac{\partial x^\mu}{\partial \hat{x}^x}, \quad [A^{-1}]_{x\mu} \equiv e^\mu_x \equiv \frac{\partial \hat{x}^x}{\partial x^\mu}, \quad (5.8)$$

we see immediately that Eq. (5.6) implies the relation

$$\hat{H} = A^T H A. \quad (5.9)$$

The Poisson bracket $\{F, G\}$ between any two scalar fields F and G on the manifold M can be written as

$$i\{F, G\} \equiv \sum_n \left(\frac{\partial F}{\partial \psi_n} \frac{\partial G}{\partial \psi_{\bar{n}}} - \frac{\partial F}{\partial \psi_{\bar{n}}} \frac{\partial G}{\partial \psi_n} \right) = \left(\frac{\partial F}{\partial x} \right)^T J \left(\frac{\partial G}{\partial x} \right), \quad (5.10)$$

in terms of the column vector $[\partial G / \partial x]_\mu \equiv \partial G / \partial x^\mu$, and the symplectic block matrix,

$$J \equiv \begin{bmatrix} 0 & 1 \\ -1 & 0 \end{bmatrix}, \quad J^2 = -I. \quad (5.11)$$

The condition that the transformation of basis is canonical is that the Poisson bracket is left invariant under the change of coordinates, and Eqs. (5.8), (5.10), and (5.11) immediately yield the necessary condition,

$$A J A^T = J. \quad (5.12a)$$

Equations (5.11) and (5.12a) readily yield the relations

$$A^{-1} = -J A^T J, \quad A^T J A = J. \quad (5.12b)$$

By making use of Eq. (5.12a), Eq. (5.9) is readily reduced to the equivalent form,

$$KA = A\mathcal{E}, \quad (5.13)$$

in terms of the matrices K and $\mathcal{E}$ defined as

$$K \equiv JH, \quad \mathcal{E} \equiv J\hat{H} = \begin{bmatrix} \varepsilon & 0 \\ 0 & -\varepsilon \end{bmatrix}. \quad (5.14)$$

Equation (5.13) is a standard eigenvalue problem. If the solution to it is written in the form

$$A = \sum_{\lambda} f_{\lambda} e_{\lambda}^T, \quad A^{-1} = \sum_{\lambda} e_{\lambda} \tilde{f}_{\lambda}^T, \quad (5.15)$$

the column vectors f_{λ} and row vectors $\tilde{f}_{\lambda}^T$ are clearly required to satisfy both the eigenvalue equations,

$$Kf_{\lambda} = \varepsilon_{\lambda} f_{\lambda}, \quad \tilde{f}_{\lambda}^T K = \varepsilon_{\lambda} \tilde{f}_{\lambda}^T, \quad (5.16)$$

where

$$\varepsilon_{\lambda} \equiv [\mathcal{E}]_{\lambda\lambda} = -\varepsilon_{\bar{\lambda}}, \quad (5.17)$$

and the normalization requirements,

$$\tilde{f}_{\kappa}^T f_{\lambda} = \delta_{\kappa, \lambda}, \quad I = \sum_{\lambda} f_{\lambda} \tilde{f}_{\lambda}^T. \quad (5.18)$$

The fact that from Eq. (5.17) the eigenvalues appear in pairs differing only in sign, is a reflection of the underlying form of K from Eq. (5.14) as the product of an antisymmetric with a symmetric matrix. It is also straightforward to prove from Eqs. (5.11), (5.16), and (5.17) that

$$f_{\lambda}^T J = n_{\lambda} \tilde{f}_{\bar{\lambda}}^T, \quad (5.19)$$

where n_{λ} is a c-number. By making further use of both the normalization condition of Eq. (5.18) and the condition of Eq. (5.12) that A represents a canonical transformation, we readily find

$$f_{\lambda}^T J f_{\bar{\lambda}} = n_{\lambda} j_{\lambda} \equiv [J]_{\lambda\bar{\lambda}} = -j_{\bar{\lambda}}. \quad (5.20)$$

Hence, $j_{\lambda} = \pm 1$, depending on whether the index λ belongs to the upper or lower half of the block matrix $\mathcal{E}$ (i.e., $j_l = +1$, $j_{\bar{l}} = -1$).

We may now define the metric g as a symmetric tensor of type (0,2), both in the coordinate and the noncoordinate bases,

$$g \equiv g_{\mu\nu} dx^{\mu} \otimes dx^{\nu} \equiv \hat{g}_{\alpha\beta} d\hat{x}^{\alpha} \otimes d\hat{x}^{\beta} \equiv \sum_a (d\hat{x}^{\hat{a}} \otimes d\hat{x}^a + d\hat{x}^a \otimes d\hat{x}^{\hat{a}}). \quad (5.21a)$$

The coefficients are, by definition, $g_{\mu\nu} \equiv g(e_\mu, e_\nu) = g(\partial_\mu, \partial_\nu)$. In terms of the usual differential length, ds , we may write

$$ds^2 = \sum_{\mu, \nu} g_{\mu\nu} dx^\mu dx^\nu = \sum_{\alpha, \beta} \hat{g}_{\alpha\beta} d\hat{x}^\alpha d\hat{x}^\beta \equiv 2 \sum_a d\hat{x}^{\hat{a}} d\hat{x}^{\hat{a}}. \quad (5.21b)$$

The constant noncoordinate basis metric matrix is thus specified as

$$\hat{g}_{\alpha\beta} = e_\alpha^T G e_\beta = [G]_{\alpha\beta} \equiv \delta_{\alpha, \beta} \Leftrightarrow G \equiv \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}. \quad (5.22)$$

In order to motivate the above metric we note that in the case of the CIM it reduces to the ordinary complex Euclidean metric, and the induced metric in the physical phase space $\Gamma_{\text{phys}}^{\text{CIM}}$ is Riemannian and positive definite. In the cases of the NCCM and the ECCM the induced metrics in the physical phase spaces, $\Gamma_{\text{phys}}^{\text{NCCM}}$ and $\Gamma_{\text{phys}}^{\text{ECCM}}$, respectively, may be complex and their physical meaning thereby not so evident.

The meaning may, however, be clarified somewhat by introducing another canonical transformation by choosing the locally diagonal coordinates $\{\hat{x}^a, \hat{x}^{\hat{a}}\}$ such that

$$d\hat{x}^a = \frac{c_a}{\sqrt{2}} (d\phi^a + i d\pi^a), \quad d\hat{x}^{\hat{a}} = \frac{1}{c_a \sqrt{2}} (d\phi^a - i d\pi^a), \quad (5.23)$$

where c_a is an arbitrary constant. The second-order Hamiltonian then becomes

$$\bar{H}_{(2)}(\phi + d\phi, \pi + d\pi) = \frac{1}{2} \sum_a \varepsilon_a [(d\pi^a)^2 + (d\phi^a)^2]. \quad (5.24)$$

It is trivial to see that the coordinates $\{\phi^a\}$ and their conjugate momenta $\{\pi^a\}$ obey the canonical Poisson bracket rules,

$$\{\phi^a, \pi^b\} = \delta_{a,b}, \quad \{\phi^a, \phi^b\} = 0 = \{\pi^a, \pi^b\}. \quad (5.25)$$

The metric in this basis is given as

$$ds^2 = \sum_a [(d\pi^a)^2 + (d\phi^a)^2]. \quad (5.26)$$

In the case of the CIM this is a global Riemannian metric in the Euclidean physical submanifold, and the coordinates and momenta are real. Precisely the same form may now also be used for both the NCCM and the ECCM, but in neither of these cases is it either global or necessarily real-valued even in the physical submanifold. The actual determination of suitable real coordinates in the physical NCCM and ECCM submanifolds is a problem that we do not consider further in the present paper.

Equations (5.21) and (5.22) lead to the relationship,

$$G = A^T g A, \quad e_\mu^T g e_\nu = [g]_{\mu\nu} \equiv g_{\mu\nu}, \quad (5.27)$$

between the non-coordinate basis metric matrix G and its coordinate basis counterpart g . By making use of Eqs. (5.11) and (5.12) and the trivial relation $JGJ = G$, Eq. (5.27) readily yields

$$g = JAG A^T J. \quad (5.28)$$

Further use of Eqs. (5.15), (5.19), (5.20), and (5.22) then yields the final expression for the metric matrix g ,

$$g = - \sum_{\lambda} j_{\lambda} J P_{\lambda}, \quad (5.29)$$

in terms of the projection matrix P_{λ} defined as

$$P_{\lambda} \equiv f_{\lambda} \tilde{f}_{\lambda}^T. \quad (5.30)$$

Before proceeding we note that the vielbein matrix A is not uniquely determined by the above considerations. For example, other valid solutions can be obtained as

$$A \rightarrow AC, \quad C = \begin{bmatrix} c & 0 \\ 0 & c^{-1} \end{bmatrix}, \quad (5.31)$$

where c is a diagonal submatrix. This freedom corresponds to the scaling of the coordinates,

$$d\hat{x}^a \rightarrow d\hat{x}^a/c_a, \quad d\hat{x}^{\bar{a}} \rightarrow c_a d\hat{x}^{\bar{a}}, \quad (5.32)$$

which leaves the second-order Hamiltonian of Eq. (5.6) invariant. Under this (canonical) transformation the metric tensor is also left invariant,

$$g = JAG A^T J \rightarrow JACGCA^T J = g, \quad (5.33)$$

since $CGC = G$.

Further valid solutions are obtained by permuting the columns of the vielbein matrix A . The permutations correspond to reordering the eigenvalues $\{\varepsilon_a\}$. Some of these transformations are not metrically equivalent. For example, a complex rotation of $\frac{1}{2}\pi$ between a particular pair of conjugate coordinates, $d\hat{x}^a \rightarrow d\hat{x}^{\bar{a}}$, $d\hat{x}^{\bar{a}} \rightarrow -d\hat{x}^a$ (which corresponds to $d\phi^a \rightarrow -i d\pi^a$, $d\pi^a \rightarrow -i d\phi^a$), is a canonical transformation under which $\varepsilon_a d\hat{x}^{\bar{a}} d\hat{x}^a \rightarrow -\varepsilon_a d\hat{x}^{\bar{a}} d\hat{x}^a$. It thus has the effect of exchanging the eigenvalues ε_a and $\varepsilon_{\bar{a}} = -\varepsilon_a$. Although this transformation is canonical, the metric matrix is not invariant under it. Combinations of this and other such canonical transformations lead to permutations of a part or all of the eigenvalues. At the ground-state point p_0 it is a simple matter to choose the set of

positive eigenfrequencies $\{\epsilon_a\}$ to define (and order) uniquely the non-coordinate basis vectors $\{\hat{e}_a\}$, and hence also to define uniquely the differential Hamiltonian of Eq. (5.6), apart from the scaling considered previously. However, at general points $p \in M$ the eigenvalues $\{\epsilon_\lambda\}$ may not be real, and hence how to choose a unique definition of the basis vectors $\{\hat{e}_a\}$ and the differential Hamiltonian is not immediately clear.

A particularly problematic feature associated with the above non-uniqueness of ordering is the possibility that on traversing a closed loop $p = p(s)$ in the state space with ground state p_0 as the base point, the non-coordinate basis (e.g., in the chart $K_{p(s)}$) may change continuously into a permuted version of the standard choice. Such an outcome would correspond to a rather complicated type of (an)holonomy. It could even result in the case where a right-handed basis returned as a left-handed one after traversing the closed loop. Such manifolds are called nonorientable. A two-dimensional example is the Möbius band. On the other hand, it is well known that finite-dimensional real symplectic manifolds are always orientable [26], since the closed $2m$ -form $dq^1 \wedge dp^1 \wedge \dots \wedge dq^m \wedge dp^m$ provides a unique positive volume measure everywhere on the $2m$ -dimensional manifold. We may hope that a similar result is also valid in the present case, at least in the physical submanifold. If this turns out not to be the case, the present metrization is problematic, and other choices might need to be considered.

We now return to Eq. (5.29) to calculate the local differential properties of the metric tensor g . On the manifold the projections P_λ and the vielbein matrix A (together with most other quantities defined, except for the constant matrices G and J , for example) depend on the specific point $p = \{x^\mu\}$ at which they are calculated in a given chart. By differentiating the eigenvalue equation (5.16) with respect to the coordinate x^μ and by using the normalization condition of Eq. (5.18), we find

$$\tilde{f}_\mu^\top K_\sigma f_\lambda = \frac{\partial \epsilon_\lambda}{\partial x^\sigma} \delta_{\mu,\lambda} + (\epsilon_\lambda - \epsilon_\mu) \tilde{f}_\mu^\top \frac{\partial f_\lambda}{\partial x^\sigma}, \quad (5.34)$$

where, consistent with the earlier notation of Eqs. (5.4) and (5.14), we define

$$K_{\sigma\tau\dots} \equiv JH_{\sigma\tau\dots}, \quad H_{\sigma\tau\dots} \equiv \frac{\partial}{\partial x^\sigma} \frac{\partial}{\partial x^\tau} \dots \bar{H}. \quad (5.35)$$

Equation (5.34) readily yields the two results, equivalent to first-order perturbation theory,

$$\frac{\partial \epsilon_\lambda}{\partial x^\sigma} = \tilde{f}_\lambda^\top K_\sigma f_\lambda, \quad (5.36)$$

$$(I - P_\lambda) \frac{\partial f_\lambda}{\partial x^\sigma} = \sum_{\mu \neq \lambda} \frac{1}{(\epsilon_\lambda - \epsilon_\mu)} P_\mu K_\sigma f_\lambda. \quad (5.37)$$

Differentiation of the normalization condition of Eq. (5.18) similarly yields the relation

$$P_\lambda \frac{\partial f_\lambda}{\partial x^\sigma} = -f_\lambda \frac{\partial \tilde{f}_\lambda^\tau}{\partial x^\sigma} f_\lambda. \quad (5.38)$$

From Eqs. (5.37) and (5.38), together with their obvious analogues for $\tilde{f}_\lambda$, it is straightforward to prove the relation

$$\frac{\partial P_\lambda}{\partial x^\sigma} = \sum_\mu \frac{1 - \delta_{\lambda,\mu}}{\varepsilon_\lambda - \varepsilon_\mu} (P_\mu K_\sigma P_\lambda + P_\lambda K_\sigma P_\mu), \quad (5.39)$$

where we also make use of the relation

$$P_\lambda \frac{\partial P_\lambda}{\partial x^\sigma} P_\lambda = 0, \quad (5.40)$$

which follows trivially from differentiating the relation $P_\lambda^2 = P_\lambda$. The second-order derivative $\partial^2 P_\lambda / \partial x^\sigma \partial x^\tau$ may now also be obtained by further differentiation of Eq. (5.39) and by making use also of Eq. (5.36). The computations involved are rather tedious and unilluminating, and we do not present the details.

Instead, we give only the final results for the first and second derivatives of the metric matrix obtained from Eq. (5.29). For simplicity, the results are written for a point where the coordinate and the non-coordinate bases coincide, namely one at which $f_\lambda \rightarrow e_\lambda$, $P_\lambda \rightarrow e_\lambda e_\lambda^\tau$ and, hence, where also the second-order Hamiltonian is diagonalized, $H_{mn} = 0 = H_{\tilde{m}\tilde{n}}$, $H_{\tilde{m}n} = \varepsilon_m \delta_{m,n} = H_{m\tilde{n}}$. By defining the quantity $D_{\mu\nu}$ as

$$D_{\mu\nu} \equiv \frac{1}{2} \frac{(j_\mu + j_\nu)}{(\varepsilon_\mu + \varepsilon_\nu)} \leftrightarrow D_{mn} = \frac{1}{(\varepsilon_m + \varepsilon_n)} = D_{\tilde{m}\tilde{n}}, \quad D_{m\tilde{n}} = 0 = D_{\tilde{m}n}, \quad \forall m, n, \quad (5.41)$$

it is possible to cast the final results in the form

$$\frac{\partial g_{\mu\nu}}{\partial x^\sigma} \xrightarrow{\text{d}} 2D_{\mu\nu} H_{\mu\nu\sigma}, \quad (5.42)$$

$$\begin{aligned} \frac{\partial^2 g_{\mu\nu}}{\partial x^\sigma \partial x^\tau} \xrightarrow{\text{d}} & 2D_{\mu\nu} H_{\mu\nu\sigma\tau} + 2 \sum_\kappa (D_{\mu\kappa} D_{\nu\bar{\kappa}} - D_{\mu\nu} D_{\mu\kappa} - D_{\mu\nu} D_{\nu\bar{\kappa}}) \\ & \times (H_{\mu\sigma\kappa} H_{\nu\tau\bar{\kappa}} + H_{\mu\tau\kappa} H_{\nu\sigma\bar{\kappa}}), \end{aligned} \quad (5.43)$$

where the symbol $\xrightarrow{\text{d}}$ indicates that the expressions are valid only at points where the second-order Hamiltonian is diagonal (i.e., at points where the coordinate and non-coordinate bases coincide). We warn the reader that a considerable amount of rearrangement of terms is necessary to obtain the final form of Eq. (5.43) in which all energy denominators of the form $(1 - \delta_{\mu,\nu})(\varepsilon_\mu - \varepsilon_\nu)^{-1}$ have been eliminated in favour of the much more regular function $D_{\mu\nu}$.

Our final aim is to study the local differential geometry of our ICM manifolds. In order to do so it is necessary to introduce a definition of parallel transport via the usual affine connection or covariant derivative. At first sight it appears tempting to use the non-coordinate basis to fix the parallel transport by demanding that the connection coefficients are chosen so that the covariant derivatives of the basis vectors $\hat{e}_\alpha$ vanish. This would ensure that two vectors, V at point p and V' at point p' , are parallel if their components in the non-coordinate bases are equal. In such a case the torsion tensor would be nonzero, while the Riemann curvature tensor would vanish, and the manifold would thus be parallelizable. It is known that such a definition for the connection succeeds globally only if there exist m vector fields (where m is the dimension of the manifold, in our case infinity) which are everywhere linearly independent [24]. However, our information on the global topology of the NCCM and ECCM manifolds is not sufficient to allow this strong assumption. Furthermore, it is difficult to know how to proceed with "flat" manifolds with torsion.

Instead, we adopt the much more familiar convention of using the coordinate basis to define a torsion-free connection, which is therefore symmetric. The further requirement of metric compatibility (namely that the inner product between two column vectors U and V , $U^T g V$, is preserved by parallel transport along any curve in the manifold) then leads, as is well known, to the unique Levi-Civita connection which is given by the Christoffel symbol,

$$\Gamma_{\mu\nu}^\kappa = \left\{ \begin{matrix} \kappa \\ \mu\nu \end{matrix} \right\} \equiv \frac{1}{2} \sum_\lambda (g^{-1})_{\kappa\lambda} \left(\frac{\partial g_{\nu\lambda}}{\partial x^\mu} + \frac{\partial g_{\mu\lambda}}{\partial x^\nu} - \frac{\partial g_{\mu\nu}}{\partial x^\lambda} \right). \quad (5.44)$$

At the points at which the coordinate and non-coordinate bases coincide, $g \rightarrow G = G^{-1}$ from Eq. (5.22), and hence by using Eq. (5.42) we have

$$\Gamma_{\mu\nu}^\kappa \xrightarrow{d} (D_{\mu\bar{\kappa}} + D_{\nu\bar{\kappa}} - D_{\mu\nu}) H_{\mu\nu\bar{\kappa}}. \quad (5.45)$$

We now adopt the standard definition of the Riemann curvature tensor,

$$R_{\kappa\lambda\mu\nu} \equiv \sum_\sigma g_{\kappa\sigma} \left[\frac{\partial}{\partial x^\mu} \Gamma_{\lambda\nu}^\sigma - \frac{\partial}{\partial x^\nu} \Gamma_{\lambda\mu}^\sigma + \sum_\tau (\Gamma_{\lambda\nu}^\tau \Gamma_{\tau\mu}^\sigma - \Gamma_{\lambda\mu}^\tau \Gamma_{\tau\nu}^\sigma) \right]. \quad (5.46)$$

For present calculational purposes, Eq. (5.46) is more conveniently recast into the equivalent form

$$\begin{aligned} R_{\kappa\lambda\mu\nu} = & \frac{1}{2} \left(\frac{\partial^2 g_{\kappa\nu}}{\partial x^\lambda \partial x^\mu} + \frac{\partial^2 g_{\lambda\mu}}{\partial x^\kappa \partial x^\nu} - \frac{\partial^2 g_{\lambda\nu}}{\partial x^\kappa \partial x^\mu} - \frac{\partial^2 g_{\kappa\mu}}{\partial x^\lambda \partial x^\nu} \right) \\ & + \sum_{\sigma, \tau} g_{\sigma\tau} (\Gamma_{\lambda\mu}^\sigma \Gamma_{\kappa\nu}^\tau - \Gamma_{\kappa\mu}^\sigma \Gamma_{\lambda\nu}^\tau). \end{aligned} \quad (5.47)$$

The once-contracted Riemann tensor, or Ricci tensor, is defined as

$$R_{\mu\nu} \equiv \sum_{\kappa, \lambda} (g^{-1})_{\kappa\lambda} R_{\kappa\mu\lambda\nu} \xrightarrow{d} \sum_{\kappa} R_{\kappa\mu\kappa\nu}. \quad (5.48)$$

By making use of Eqs. (5.43) and (5.45) it is readily evaluated in the present case at a point where the coordinate and non-coordinate bases coincide as

$$\begin{aligned} R_{\mu\nu} \xrightarrow{d} & \sum_{\kappa} H_{\nu\kappa\kappa} (D_{\mu\kappa} + D_{\nu\kappa} - D_{\mu\nu}) + \sum_{\kappa, \lambda} H_{\mu\nu\lambda} H_{\kappa\bar{\kappa}\bar{\lambda}} [2D_{\mu\nu} D_{\kappa\bar{\lambda}} \\ & - D_{\kappa\bar{\lambda}} (D_{\mu\bar{\lambda}} + D_{\nu\bar{\lambda}}) - D_{\bar{\kappa}\bar{\lambda}} (D_{\mu\kappa} + D_{\nu\kappa}) - D_{\mu\kappa} D_{\mu\bar{\lambda}} - D_{\nu\kappa} D_{\nu\bar{\lambda}}] \\ & + \sum_{\kappa, \lambda} H_{\mu\kappa\lambda} H_{\nu\bar{\kappa}\bar{\lambda}} [2D_{\mu\nu} (D_{\mu\kappa} + D_{\nu\bar{\lambda}}) - 2D_{\mu\kappa} D_{\nu\bar{\lambda}} + D_{\kappa\bar{\lambda}} (D_{\mu\kappa} + D_{\nu\bar{\lambda}}) \\ & - D_{\kappa\bar{\lambda}} (D_{\mu\bar{\lambda}} + D_{\nu\kappa}) - D_{\mu\kappa} D_{\mu\bar{\lambda}} - D_{\nu\bar{\lambda}} D_{\nu\kappa} - D_{\kappa\bar{\lambda}}^2]. \end{aligned} \quad (5.49)$$

Finally, the scalar curvature is defined as

$$R \equiv \sum_{\mu, \nu} (g^{-1})_{\mu\nu} R_{\mu\nu} \xrightarrow{d} \sum_{\mu} R_{\mu\bar{\mu}}. \quad (5.50)$$

After some simplification we readily obtain the final result,

$$\begin{aligned} R \xrightarrow{d} & 4 \sum_{m, n} H_{\bar{m}\bar{n}mn} D_{mn} - 4 \sum_{m, n, l} H_{\bar{m}ml} H_{\bar{l}nn} (D_{ml} D_{nl} + D_{mn} D_{ml} + D_{mn} D_{nl}) \\ & - 2 \sum_{m, n, l} H_{\bar{l}mn} H_{\bar{m}\bar{n}l} (D_{mn}^2 + 4D_{mn} D_{nl}) - 2 \sum_{m, n, l} H_{\bar{m}\bar{n}l} H_{mnl} D_{mn}^2. \end{aligned} \quad (5.51)$$

We remind the reader that Eqs. (5.49) and (5.51) are valid at every point p around which the second-order part of the Hamiltonian is diagonalized, i.e., such that (and compare Eq. (3.42))

$$\begin{aligned} \bar{H} \xrightarrow{d} & H_0 + \sum_{n=1}^{\infty} (H_n \psi_n + H_{\bar{n}} \psi_{\bar{n}}) + \sum_{n=1}^{\infty} \varepsilon_n \psi_{\bar{n}} \psi_n \\ & + \sum_{\substack{m=0 \\ (m+n \geq 3)}}^{\infty} \sum_{n=0}^{\infty} \frac{1}{m! n!} \sum_{\bar{m}_1=1}^{\infty} \cdots \sum_{\bar{m}_m=1}^{\infty} \\ & \times \sum_{n_1=1}^{\infty} \cdots \sum_{n_n=1}^{\infty} H_{\bar{m}_1 \cdots \bar{m}_m n_1 \cdots n_n} \times \psi_{\bar{m}_1} \cdots \psi_{\bar{m}_m} \psi_{n_1} \cdots \psi_{n_n}. \end{aligned} \quad (5.52)$$

The components of the Ricci tensor and the various terms of the scalar curvature are illustrated schematically in Figs. 1 and 2, respectively. Although these diagrams are not in any sense directly related to Goldstone or Feynman diagrams, their qualitative structure is apparent by comparison with the respective equations (5.49)

FIG. 1. Diagrams illustrating the terms that contribute to the Ricci tensor, as described in the text.

and (5.51). However, we make no attempt here to derive quantitative rules for the evaluation of such diagrams.

There are now several points of interest which emerge from the above analysis. We first consider the simplest of the three ICM representations, namely the CIM. This has an integrable bilinear Hamiltonian, from Eq. (3.3), and it is trivial to see from Eqs. (5.43), (5.45), and (5.47) that the affine connection and the Riemann tensor vanish identically in this case. This is hardly surprising since it was precisely our intention that the CIM phase space should be regarded as flat in our metrization. Indeed, we recognized from the outset that the CIM phase space, Γ^{CIM} , is a complex Euclidean space, which can be covered by a single chart.

A somewhat less expected result is that the curvature of the NCCM manifold Γ^{NCCM} is also zero by our convention. This is simply seen if we observe that every term in Eq. (5.51) involves a matrix element of the Hamiltonian with at least two tilde indices, whereas the NCCM Hamiltonian of Eq. (3.21) is at most of first order in the tilde coordinates. Thus, although of the two operators $\{S, \tilde{S}\}$ which characterize the NCCM, the operator S appears nonlinearly, it would appear that the remaining linearity which characterizes the use of $\tilde{S}$ is sufficient to retain the zero curvature of the manifold Γ^{NCCM} . Thus, although the Riemann and Ricci tensors do not vanish identically in Γ^{NCCM} , the NCCM phase space is still essentially flat.

Finally, we note that of the three ICM parametrizations, only the ECCM is fully nonlinear in both operators, $\{\Sigma, \tilde{\Sigma}\}$, which fully parametrize the states $\{|\Psi\rangle, \langle\tilde{\Psi}|\}$. Furthermore, we now observe from Eq. (5.51) that only this case is fully nontrivial in the sense that the curvature of its associated phase space, Γ^{ECCM} , may be nonzero. This is formally obvious because the diagonalized ECCM Hamiltonian has terms in the expansion of Eq. (5.52) of arbitrarily high order in both the tilde and the non-tilde coordinates. In order to prove that the Hamiltonian matrix elements are such that the curvature does not in fact vanish identically everywhere, it should suffice in broad terms to point out that the fourth-order ECCM matrix elements $H_{\tilde{m}\tilde{n}mn}$ appearing in Eq. (5.51) cannot be given wholly in terms of the eigenfunctions and eigenenergies, unlike the remaining third-order elements which can be so given, as was demonstrated in Section III (and see

FIG. 2. Diagrams for the scalar curvature in the present metrization.

Eqs. (3.47a)–(3.47d)). The fourth- and higher-order Hamiltonian matrix elements depend explicitly on the potential function U , as was pointed out in Section III, and they cannot generally be simplified to the extent of eliminating any specific reference to it. It would take us too far afield at present to dwell upon the detailed proofs of both the above point and the convergence of the infinite summations in the above expressions for the Riemann and Ricci tensors and the scalar curvature. Preliminary investigations strongly indicate that they do all properly converge, whence the Riemann tensor and curvature are finite-valued and nonzero. Thus, despite its enormous complexity, it would appear that at least in this respect the ECCM manifold resembles a more ordinary finite-dimensional manifold.

We note that in the Riemannian geometry of finite-dimensional manifolds, a scalar such as the curvature does not depend on the coordinate system used to calculate it. Similarly, if a tensor vanishes at a point in a given chart, it vanishes in all other charts. It is therefore clear that the nonlinear canonical transformations from the CIM to the NCCM and, further, to the ECCM are, in the present infinite-dimensional case, topologically more drastic than any usual coordinate transformation. They involve a mathematically singular mapping that cannot be obtained from the identity in a continuous fashion because of some topological obstruction. Indeed, the distributions of these zeros for various states are closely related to the homology and homotopy structure of the manifold as a topological space. These aspects, together with the associated cohomology structure of the differential forms defined on the manifolds, certainly deserve a detailed and quantitative understanding.

We end this section by attempting to develop some overall qualitative view of the geometry of the ECCM manifold Γ^{ECCM} in the metrization outlined above. In the first place, we have no particular reason to expect that the differential geometries at the replica points p' of a given physical state in the corresponding charts K' , are identical. Thus, the charts may indeed represent intrinsically inequivalent canonical representations of the neighbourhood of a state. A partial explanation of this phenomenon may be that the canonical generalized coordinates are not themselves physical observables, as was explained in some detail in II (and see, particularly, Section V.2 of II). However, quantities such as $\bar{H}$ and its one-form, $d\bar{H}$, are physical observables, and they must be invariant at different replicas of the same physical point. The same is true for all functions $f \in \mathcal{F}^c(M) \subset \mathcal{F}(M)$, where, as explained in Section V.2 of II, $\mathcal{F}^c(M)$ is the function subspace of observables on the ECCM manifold $M \equiv \Gamma^{\text{ECCM}}$, and $\mathcal{F}(M)$ is the space of all (sufficiently smooth) functions on M . We showed in II that for an observable $\bar{A} \equiv \bar{A}[\psi_n, \psi_{\bar{n}}] \in \mathcal{F}(M)$ actually to represent the average value of an operator $A \in \mathcal{H}$, the original Hilbert space, (i.e., so that $A \in \mathcal{F}^c(M)$), certain consistency relations involving derivatives of $\bar{A}$ up to second order need to be satisfied.

It is interesting to enquire whether the scalar curvature R of the ICM phase spaces, for example, is also a physical observable in the above sense. The consistency conditions in this case clearly involve derivatives of $\bar{H}$ up to sixth order with respect to the coordinates $\{\psi_n, \psi_{\bar{n}}\}$, and we have not yet undertaken the

somewhat daunting task of investigating them. If the curvature does turn out to be a physical observable, then its value will be the same in all charts K' . In this case it may then be possible to view each of the replica points as being the *same* physical point in the ECCM phase space, up to some equivalence, even though the coordinates have changed continuously to new values rather than recovering their original values. A closed loop in the state space would then effectively be mapped into a closed loop in the ECCM phase space, but going around a "neck" or through a "handle" of the geometry. In turn, this would imply that many (indeed almost all) of the dimensions are compactified. It is clear that the above picture is still far from complete and that more work remains to be done. For example, it is far from clear as yet how the states that are not CC-representable would actually show up in the manifold.

VI. SUMMARY AND DISCUSSION

In this paper we have given a rather extensive and mathematically rigorous treatment of the anharmonic oscillator considered as a model $(0+1)$ -dimensional quantum field theory described by the apparatus of coupled cluster theory. We believe that this application is the first nontrivial case with an infinite-dimensional Hilbert space that has been studied to this depth by both the normal (NCCM) and extended (ECCM) versions of the theory or, for that matter, by any alternative formulation of quantum many-body theory. For this particular example we know a great deal about the exact solutions to the Schrödinger equation (which is, of course, why the model was chosen for detailed study in the first place), and these have been fully utilized in our treatment. A principal tool has been to work within the Bargmann Hilbert space. This has enabled us to give precise meaning to many concepts or entities that are extremely problematic within the usual formulation of functional analysis. Examples include unbounded operators, operators with empty domain, and non-normalizable state vectors, all of which arise naturally and necessarily within the coupled cluster analysis of infinite-dimensional bosonic systems.

This third paper in a series devoted to these topics has focussed especially on the geometrical structure of the CCM phase spaces. We note that these are actually "superspaces" in the sense that each point in the phase space represents a complete description of the quantum-mechanical pure state. They represent mappings of the Hilbert space. More particularly, they are classical symplectic manifolds in which the dynamics is determined by the mapped, classicized Hamiltonian, which is itself simply the expectation value of the quantum-mechanical Hamiltonian expressed in terms of the CCM canonical coordinates. The present phase spaces, Γ^{CCM} , are infinite-dimensional manifolds, and as such many of the standard theorems concerning finite-dimensional manifolds are inapplicable.

At the ground-state point p_0 of each CCM phase space, we introduced the normal-coordinate system and derived the nonlinear expansion for the average

value $\bar{H}$ of the quantum-mechanical Hamiltonian in its neighbourhood. The quadratic part (i.e., terms up to second order in the normal coordinates $\{\psi_n, \tilde{\psi}_n\}$) of the average-value functional $\bar{H} = \bar{H}[\psi_n, \tilde{\psi}_n]$ is sufficient to determine the linear response of the system to arbitrary (infinitesimal) perturbations, although the higher-order nonlinear terms are naturally required in the case of stronger perturbations. We also considered similar normal-mode expansions around other points in the phase space, but explicit constructions were only given at the ground-state point p_0 for the coefficients in these expansions.

We have shown that the CCM phase spaces are manifolds with complicated topological structure. They display (an)holonomies of various kinds. For example, a closed smooth loop in the Hilbert space may be mapped into an open smooth loop in the mapped phase space, with different values for the coordinates of the starting and end points, using the continuation of the same chart. We showed that this type of holonomy is $\sim \mathbb{Z}$, due to the fact that a given state can have a countably infinite number of "replicas" within the phase space. Each such replica is reachable from any other by a smooth path. Hence, the phase space is connected, although it is not necessarily simply connected.

In order to investigate the geometrical structure more deeply we next introduced a natural metric on the phase space. This is based on the local normal coordinate system at each point, and as such is wholly determined by the Hamiltonian of the system. In doing this, all degrees of freedom were treated on an equal footing and taken as coordinates in the base space. Thus, no fibres were left over and above the tangent space. Hence, in this particular (geo)metrization geodesics clearly cannot be trajectories. This is evident, because if both "coordinates" and "momenta" are chosen as coordinates in the manifold, there can be only one trajectory through each point, whereas geodesics can go in an arbitrary direction from a given point. We note in passing that it might be interesting to study alternative choices. Particularly interesting would be geometries in which the geodesics and trajectories do coincide. A possible way to achieve this might be by performing a suitable Legendre transformation from the Hamiltonian to the Lagrangian structure at each point of the phase space, thereby reducing the dimensionality of the base space by one-half, taking time as an additional local coordinate direction, and introducing a suitable metric in the resulting "configuration-space-plus-time" manifold.

Nevertheless, the great advantage of the present choice of metric is that the phase space of the primitive so-called configuration interaction method (CIM) turns out to be flat. It is simply the infinite-dimensional complex Euclidean space, which is also a Kähler manifold. On the other hand, the NCCM phase space also has zero curvature, although its Riemann and Ricci tensors do not vanish identically. Finally, the ECCM phase space has nonzero values for each of the scalar curvature and the Riemann and Ricci tensors.

While we have been able to be rather precise in our discussion of the differential geometry of these ICM phase spaces, our discussion of their global structure or topology has necessarily been somewhat speculative. However, it does appear that an interpretation is possible of the various replicas within the mapped ECCM

phase space of the same point in the original Hilbert space, whereby these replicas can be regarded in some sense as the *same* point on the manifold. If this is correct, going smoothly from a given replica point p^1 to another p^2 corresponding to the same physical state, would represent going around a "neck" or through a "handle" back to the same place.

The above mental image is possible only if the manifold is thought to be embedded in a higher-dimensional Euclidean space and its metric to be the induced metric. Because of intervening topological obstructions, caused in the present case by the zeros of the Bargmann wave function, these loops cannot be shrunk into points, and the manifold thereby becomes multiply connected with genus equal to infinity. Other complicating aspects derive from the existence of states that are not representable by the coupled-cluster parametrizations. We have not explored how such states are mapped into the CCM phase spaces. One hope and possibility is that they are mapped into points which are infinitely far away (from, say, p_0) if measured by our adopted metric.

In order to obtain some feeling for our somewhat abstract analysis, it is useful to consider a simple finite-dimensional example. A particularly amusing but illustrative such example is provided by the two-dimensional phase space of the original anharmonic oscillator considered in II, but now treated as a *classical* Hamiltonian. A concrete example (and see Eqs. (3.1) and (3.9) of II) is the classical quartic anharmonic oscillator,

$$\bar{H} = \frac{1}{2} p^2 + \frac{1}{2} x^2 + kx^4. \quad (6.1)$$

Clearly, the usual canonical coordinates (x, p) cover the entire two-dimensional phase space, which is therefore flat in the usual metric, and the approach adopted in the present paper is wholly unnecessary here. However, if we do adopt the metric of Section V, it is not difficult to show that the two-dimensional phase space becomes curved. The Hamiltonian $\bar{H}$ of Eq. (6.1) is first trivially put into diagonal form in the sense of Section V by the normal coordinates ψ_1 and $\psi_{\bar{1}}$ defined as

$$x \equiv \frac{1}{\sqrt{2}} (\psi_{\bar{1}} + \psi_1), \quad p \equiv \frac{i}{\sqrt{2}} (\psi_{\bar{1}} - \psi_1), \quad (6.2)$$

in terms of which we have

$$\bar{H} = \psi_{\bar{1}} \psi_1 + \frac{k}{4} (\psi_{\bar{1}} + \psi_1)^4. \quad (6.3)$$

It is now straightforward to apply the analysis of Section V at arbitrary points of the phase space to derive the phase space metric,

$$ds^2 = \sqrt{1 + 12kx^2} dx^2 + \frac{1}{\sqrt{1 + 12kx^2}} dp^2, \quad (6.4)$$

which, furthermore, can be shown to have scalar curvature given by

$$R = \frac{12k(1 - 24kx^2)}{(1 + 12kx^2)^{5/2}}. \quad (6.5)$$

If the above (two-dimensional) surface is embedded in three-dimensional Euclidean space and the induced metric is used, the manifold becomes an axisymmetric surface obtained by the rotation of a fixed curve around a symmetry axis. The surface is also reflection symmetric with respect to a plane perpendicular to the symmetry axis. The x -coordinate increases on the surface along the axial direction, and the p -coordinate increases along the azimuthal direction. The surface is wrapped infinitely many times around the symmetry axis, and it extends to infinity with monotonically decreasing radius along both axial directions. The maximum radius at the symmetry plane is a free parameter, which, however, cannot exceed the limiting value $r_{\max} = 3/2 \sqrt{k}$. As a matter of fact, the surface is obtained by an area-preserving deformation from the original planar (x, p) -surface. Although this is a most unrealistic example, it does show that the geometry is still simply connected and coverable by only one chart and that the manifold is neither closed nor of finite volume (i.e., surface area in this case).

Upon quantization of the classical one-component anharmonic oscillator, its corresponding two-dimensional phase space considered as a geometrical object is transformed within the coupled-cluster parametrization into another geometrical object with a countably infinite number of dimensions. This new manifold, particularly within the ECCM, displays many complicated geometrical features. However, if the effective compactification of many of these dimensions can be rigorously proven, the new manifold Γ^{ECCM} still has the capability to be effectively simplified.

We might now attempt to imagine how this new infinite-dimensional nonlinear classical system described by $\bar{H}^{\text{ECCM}}$ in Γ^{ECCM} could be quantized again and what the characteristics of the resulting ECCM manifold might be. To the best of our knowledge, this problem of "third quantization" has not received much attention in the literature (although the interested reader is referred to Ref. [27]). Also, the problem of quantizing a system on a curved symplectic space with possible handles and other nontrivial geometrical features is, naturally, much more complicated than the present problem. Nevertheless, the intriguing possibility suggests itself that upon successive re-quantizations in the above sense, some special particular infinite-dimensional systems described by a Hamiltonian functional over some given phase space might not change at all. Such geometrical objects would therefore be "fixed points" of quantization [18], which could equally well be described classically or quantum-mechanically in the sense that both descriptions would be identical. As a quantum theory the fixed point is free of anomalies. This feature is desirable for the fundamental theories not only of high-energy physics, where one of the main themes in recent years has been the demand that anomalies must be renormalisable, but also of the quantum theory of gravity, where the goal is to avoid, altogether, any anomalies.

We conclude by wondering what the present example of single-mode bosonic field theories can teach us about more realistic field theories in $(d+1)$ dimensions, with $d \neq 0$. As was pointed out earlier, their precise mathematical structure is still unknown, and it is only fair to point out to the reader the complexities that lie ahead, not the least of which is the extension of the present analysis to functions of several complex variables or to complex functionals. Nevertheless, we also counterbalance this warning with the remark that the NCCM and ECCM versions of the coupled-cluster theory have already been formulated and even numerically applied in low-order truncations. As an example we mention the pioneering studies of the one-dimensional ϕ^4 field theory by Kümmel and coworkers [28, 29], using the standard CCM. On the basis of the very general properties of the fully linked CC version in the ECCM, we venture to suggest the following scenario as an interesting possibility.

The original classical field theory to be quantised is typically built out of fields $\varphi_\lambda(x)$ where x is a continuum variable belonging to some noncompact d -dimensional manifold M^d , and λ belongs to a discrete and thus countable set of indices related to a number of "internal" symmetries. The pair (x, λ) is a member of the index or label set $\mathcal{J}$ discussed in I and in Refs. [18–19]. On quantisation, the connected coupled-cluster amplitudes will be of the form $\sigma_{\lambda_1 \dots \lambda_n}^{(n)}(x_1 \dots x_n)$, and the cluster property requires the positions $x_1 \dots x_n$ to be "close" to each other in order for the amplitude to be nonzero. Such functions can, under favourable circumstances, be expanded in terms of a suitable set of fields $\{\phi_A(R)\}$, where $R \in M^d$ represents the common translational degrees of freedom of the sets $\{x_1 \dots x_n \mid n=1, 2, \dots\}$, and A represents all the countable degrees of freedom arising partly from the original $\{\lambda\}$ and partly from the bound-state-like relative internal spatial modes of the clusters. The pairs (R, A) span the image of the label space $\mathcal{J}$. A fixed point would be a system for which the image of the label space can be chosen identical to the original $\mathcal{J}$ and the Lagrangian or Hamiltonian in terms of the fields $\phi_A(R)$ has the same form as originally in terms of $\varphi_\lambda(x)$. Although the quantization of a realistic field theory leads to a Hilbert space (or ICM phase space) which, naively thinking, typically has a much higher dimensionality than the original, the above scheme, which is based on the full linkedness of the additively separable cluster amplitudes, may lead one to expect that it does not always have to be so.

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