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Independent-cluster methods as mappings of quantum theory into classical mechanics*

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Summary. The algebraic structures of the *configuration interaction*, *normal coupled cluster*, and *extended coupled cluster* methods are reviewed and developed. These methods are pointed out to perform a mapping of the quantum mechanical problem into a classical phase space, where in each case the classical canonical coordinates have characteristically different cluster and locality properties. Special focus is given to the extended coupled cluster method (ECCM), which alone is based on an entirely additively separable coordinate system. The general principles are formulated for systems with both bosonic and fermionic degrees of freedom, allowing both commutative and anticommutative (Grassmann) cluster amplitudes. The properties of the classical images are briefly discussed. It is proposed that phase spaces may exist which are fixed points of quantization.

Key words: Coupled cluster theory – Extended coupled cluster method – Phase space – Additive separability – Holomorphic wave function – Bargmann Hilbert space – Grassmann algebra – Field theory – Anomalies

1. Introduction

The *configuration interaction*, *normal coupled cluster*, and *extended coupled cluster* methods (CIM, NCCM, and ECCM, respectively) are parametrizations of the many-body wave function which share the following important property. The ket and bra trial states are given in terms of two mutually commuting sets of operator amplitudes $(\tilde{X}, X)$ that belong to the subalgebras of annihilation and creation operators, respectively. These *independent cluster* (IC) methods can be formulated variationally using a quantum mechanical action principle whereby an expectation value functional for the properties is introduced. The dynamics of the IC amplitudes are obtained from equations formally identical to classical

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canonical equations of motion. The methods have their roots in nuclear physics, quantum chemistry and condensed matter physics, where they have been widely used to quantitatively and accurately describe various many-body properties (for reviews see e.g. [1–6]).

The IC parametrizations perform a "supercoherent" mapping of the Hilbert space into a "target" classical phase space, $\mathscr{H} \to coh(\mathscr{B}^{\mathscr{H}}) \sim scoh(\mathscr{H}) = \Gamma^{\mathscr{H}}$. Here $coh(\mathscr{B}^{\mathscr{H}})$ is the subset of the coherent states of an enlarged "bosonized" and "fermionized" Hilbert space $\mathscr{B}^{\mathscr{H}}$ into which $\mathscr{H}$ is embedded, and $scoh(\mathscr{H}) = \Gamma^{\mathscr{H}}$ is the mapped classical phase space. This is a valid description for each IC method. Differences show up in the qualitative nature of the amplitudes, in particular in their locality (quasilocality or multilocality) properties, which are closely connected with the extensivity or separability features of the methods or their approximants. In CIM and IC amplitudes $(\tilde{X}, X) = (\tilde{F}, F)$ are multiplicatively separable; in NCCM the amplitudes are $(\tilde{X}, X) = (\tilde{S}, S)$, of which S is additively and $\tilde{S}$ multiplicatively separable; in ECCM both of the amplitudes $(\tilde{X}, X) = (\tilde{\Sigma}, \Sigma)$ are additively separable. *Multiplicative* or *additive separability* [7] are terms which are used to describe how a particular function decomposes when the system divides into uncorrelated subsystems for example due to a large distance between them. In approximative calculations the associated *extensivity* (size-extensivity) or *size-consistency* [8–10] features are usually not automatically guaranteed.

The present article concentrates mostly on the general formulation of the ECCM. The expectation value functional is introduced in terms of bosonic commutative and fermionic anticommutative (Grassmann) cluster amplitudes. The latter facilitate the algebraic treatment of fermionic many-body systems and their fermionic excitations. Much of the technical structure of the IC methods and the ECCM are explained in Sects. 2–4 and in Appendices A–C. Excited states and transition amplitudes are treated in Sect. 5. Equations of motion and the limit of small oscillations around a stationary point are considered in the next two sections. It is shown that e.g. (anti)commutators of operators are mapped into classical (graded) Poisson brackets. Section 8 briefly discusses the possible "bugs" of the CC methods, i.e. mathematical subtleties such as convergence problems and difficulties in formulating practical truncation schemes in various applications. Section 9 is dedicated to a discussion of the classical mappings induced by the IC methods. Section 10 contains a few concluding remarks and raises the question whether the phase space description in terms of additively separable coordinates can be elevated to a more fundamental status of a new physical principle, by suggesting the possibility of fixed points of quantization.

The notation in the present article differs to some extent from the earlier conventions and is largely in accordance with a forthcoming paper written with Bishop [11].

2. Basic operator algebra

It is assumed that all states of the Hilbert space $\mathscr{H}$ can be generated from the *cyclic* vector(s) $|0\rangle$ or $\langle 0|$ by operations with the elements of the algebras $\mathscr{C}^+$ or $\mathscr{C}^-$ of *creation* or *annihilation* operators, respectively. The cyclic state (reference or model state, "vacuum") may typically be a boson vacuum, a Slater determinant or a BCS ground state. Let the indices $p, q, r, \ldots \in \mathscr{I}_1$ denote the *single-*

particle states and $\mathscr{I}_1$ the single-particle index space. The single-particle creation and destruction operators are $\{a_p^\dagger : p \in \mathscr{I}_1\}$ and $\{a_p : p \in \mathscr{I}_1\}$, respectively. They are assumed to obey the standard boson or fermion commutation or anticommutation rules. For a mixture of particles, let each index p be supplied with a "Grassmann bit" which tells whether the single-particle operator in question is bosonic or fermionic. The graded commutation rules are standard:

$$\begin{aligned} [a_p, a_q] &\equiv a_p a_q - \eta_{p,q} a_q a_p = 0, \\ [a_p, a_q^\dagger] &\equiv a_p a_q^\dagger - \eta_{p,q} a_q^\dagger a_p = \delta(p, q), \end{aligned} \tag{1}$$

with the sign factors obeying the convention $\eta_{p,q} = -1$ for $pq = FF$ and $\eta = 1$ for the other cases BB, BF, FB. The sign factors are conveniently represented in the form:

$$\eta_{p,q} = (-1)^{P_p P_q}, \tag{2}$$

where $P_p = 0 \pmod 2$ for bosonic p and $P_p = 1 \pmod 2$ for fermionic p. The fermionic parity is defined as:

$$\eta_p \equiv \eta_{p,p} = (-1)^{P_p} = \begin{cases} 1, & p = B, \\ -1, & p = F. \end{cases} \tag{3}$$

Continuous field theories necessitate continuous single-particle indices, in which case the Kronecker delta is replaced by the Dirac delta. Trivial modifications would also appear elsewhere in the subsequent discussion.

Multiparticle or *configuration* operators are generated by the single-particle operators. They span the algebras $\mathscr{C}^+$ and $\mathscr{C}^-$. It is convenient to choose them normalized,

$$C_I^\dagger = \prod_{p\rightarrow} \left[\frac{1}{\sqrt{m_p!}} (a_p^\dagger)^{m_p(I)} \right]. \tag{4}$$

The arrow denotes a definite prescribed ordering of the factors in the product. The exponents m_p can be $\{0, 1\}$ or $\{0, 1, 2, \ldots\}$, depending on if p is fermionic or bosonic. Normalization is therefore:

$$\langle 0 | C_I C_J^\dagger | 0 \rangle = \delta(I, J). \tag{5}$$

The configuration indices $\{I, J, K, \ldots\}$ are elements in the *configuration index space* $\mathscr{I}$, and the set $\{C_I^\dagger |0\rangle : I \in \mathscr{I}\}$ forms an orthonormal basis for $\mathscr{H}$. Using this basis it will be useful to express the identity operator as the resolution:

$$I^{op} = \sum_J C_J^\dagger |0\rangle\langle 0| C_J = |0\rangle\langle 0| + \sum_J{}' C_J^\dagger |0\rangle\langle 0| C_J, \tag{6}$$

where the primed summation excludes the null configuration.

The parity factors η are defined for arbitrary configuration operators by:

$$\eta_I = (-1)^{P_I} = (-1)^{\sum_p m_p(I) P_p} = (-1)^{N_F}, \tag{7}$$

where N_F is the number of fermions in configuration I. Indeed, $\eta_{A,B}$ can be similarly generalized for arbitrary operators $A, B, \ldots$.

Corresponding to each configuration index a pair of numbers $I \mapsto (\tilde{x}_I, x_I)$ are defined such that for bosonic I (i.e. $\eta_I = 1$) the $(\tilde{x}_I, x_I)$ are complex numbers,

but for fermionic I (i.e. $\eta_I = -1$) the $(\tilde{x}_I, x_I)$ are *complex Grassmann numbers* (to be more precise, they are generally even or odd elements of a complex Grassmann algebra). Their graded commutation rules with each other and with the configuration operators are defined in accordance with the usual convention (see e.g. [12, 13]) as follows:

$$\begin{aligned} &[x_I, x_J] \equiv x_I x_J - \eta_{I,J} x_J x_I = 0, \\ &[x_I, \tilde{x}_J] = [\tilde{x}_I, \tilde{x}_J] = 0, \\ &[x_I, C_J] = [x_I, C_J^\dagger] = [\tilde{x}_I, C_J] = [\tilde{x}_I, C_J^\dagger] = 0. \end{aligned} \tag{8}$$

By this choice, expressions of the form:

$$\sum_I C_I^\dagger x_I, \quad \sum_I \tilde{x}_I C_I$$

have an *even* Grassmann partity, i.e. they commute with all Grassmann numbers. The restriction to such cases follows from the convention adopted here that the Hamiltonian is always assumed to be Grassmann-even. Usually the many-body Hamiltonian contains only products of an even number of fermionic configuration operators multiplied by ordinary complex numbers, and is able to change fermion number only in multiples of two. However, for the purpose of calculating odd fermionic Green functions, correlation functions or excited states, it is very convenient to formally break the fermionic parity of H, e.g., by adding source terms of the form:

$$\sum_p (\tilde{v}_p a_p + a_p^\dagger v_p).$$

If the coefficients v, $\tilde{v}$ are chosen Grassmann numbers for each fermionic index p, the Hamiltonian still remains Grassmann-even. The IC amplitudes of the wave functions (to be described below) then become multinomials of $\{\tilde{v}_p, v_p\}$. For most purposes it will be sufficient to expand various properties only up to at most second order in the Grassmann sources.

The *derivatives* with respect to the amplitudes $(\tilde{x}_I, x_I)$ are defined to be *left* derivatives, following the standard convention [12, 13]. The following notations will be used:

$$\begin{aligned} \frac{\partial}{\partial \tilde{x}_I} &\equiv \frac{\delta}{\delta \tilde{x}_I} \equiv \partial_I, \\ \frac{\partial}{\partial x_I} &\equiv \frac{\delta}{\delta x_I} \equiv \hat{\partial}_I. \end{aligned} \tag{9}$$

The derivatives act to the right removing a factor from the left end of a product, without changes of sign. To be able to do so, the factors in a product must be rearranged using proper graded commutation rules. For example:

$$\partial_I(\tilde{x}_I \tilde{x}_J \cdots x_K) = \tilde{x}_J \cdots x_K,$$

but

$$\partial_J(\tilde{x}_L \cdots x_K x_J x_I) = \eta_{K,J} \cdots \eta_{L,J} \tilde{x}_L \cdots x_K x_I.$$

The derivatives have graded commutation rules with each other similar to those of the amplitudes.

3. Independent-cluster parametrizations of the many-body wave function

Each IC method is defined in terms of a canonically conjugate pair of operators $(\tilde{X}, X)$:

$$X = \sum_I C_I^\dagger x_I \in \mathscr{C}^+,$$
$$\tilde{X} = \sum_I \tilde{x}_I C_I \in \mathscr{C}^-. \tag{10}$$

They parametrize the ket and bra states in characteristically different ways. The cases are treated separately.

3.1. Configuration interaction method (CIM)

The states are defined as:

$$|\Psi\rangle = F|0\rangle = \sum_I C_I^\dagger |0\rangle f_I,$$
$$\langle\tilde{\Psi}| = \langle 0|\tilde{F} = \sum_I \tilde{f}_I \langle 0|C_I. \tag{11}$$

In this case $(\tilde{X}, X) = (\tilde{F}, F)$.

The average value functional for the energy can be written in the straightforward way:

$$\langle H\rangle \equiv \langle\tilde{\Psi}|H|\Psi\rangle = \sum_{IJ} \tilde{f}_I \langle I|H|J\rangle f_J. \tag{12}$$

Figure 1 illuminates the average value functional and the matrix elements:

$$\langle I|H|J\rangle = \langle 0|C_I H C_J^\dagger|0\rangle. \tag{13}$$

It turns out that the ground state amplitudes f and $\tilde{f}$ are both *disconnected.* Their values can be obtained by the Rayleigh–Ritz variational principle, where Lagrange multipliers must be used due to lack of manifest normalization:

$$\frac{\partial}{\partial \tilde{f}_I}(\langle\tilde{\Psi}|H|\Psi\rangle - \mu\langle\tilde{\Psi}|\Psi\rangle) = 0,$$
$$\frac{\partial}{\partial f_I}(\langle\tilde{\Psi}|H|\Psi\rangle - \mu\langle\tilde{\Psi}|\Psi\rangle) = 0.$$

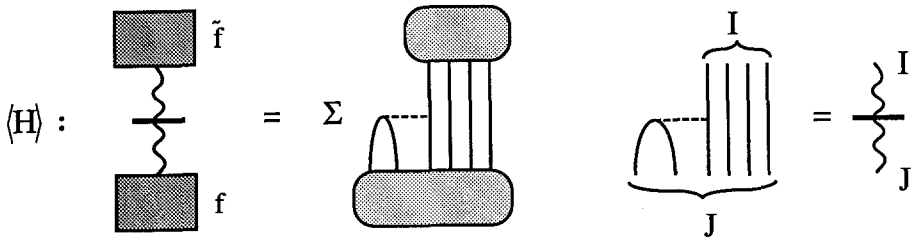

Fig. 1. Schematic presentation of the average value functional and a typical matrix element in CIM

Let the Hamiltonian be written as:

$$H = T + V; \qquad T = \sum_p a_p^t t_p a_p, \tag{14}$$

where T is the diagonal model Hamiltonian and t_p are the model single-particle energies. Above the order of the factors is chosen to facilitate the possibility of derivative operations. Then:

$$\langle H \rangle \equiv \bar{H}[\tilde{f}, f] = \bar{T} + \bar{V}, \tag{15}$$

where, in particular:

$$\bar{T} = \sum_I \tilde{f}_I T_I f_I; \qquad T_I = \sum_p m_p(I) t_p \tag{16}$$

is the diagonal part. The first variational conditions give the equations (notice that $\mu = E_0 =$ the full ground state energy):

$$T_I f_I + \frac{\partial \bar{V}}{\partial \tilde{f}_I} = E_0 f_I.$$

Symmetric equations hold for $\tilde{f}$. Iteration of these equations leads to the *Brillouin–Wigner perturbation theory*, which has its well known drawbacks for a many-body system (such as non-extensive terms in the energy expansion, etc.).

The *Rayleigh–Schrödinger perturbation theory* is recovered by replacing $V \to V' = V - E_0 I^{op}$. The stationary conditions are then:

$$\begin{aligned} f_I &= -\frac{1}{T_I} \frac{\partial \overline{V'}}{\partial \tilde{f}_I}, \\ \tilde{f}_I &= -\frac{\eta_I}{T_I} \frac{\partial \overline{V'}}{\partial f_I}. \end{aligned} \tag{17}$$

Notice that now the energy denominators T_I are *on energy shell*. The equations can be iterated to produce a diagrammatic expansion for the amplitudes and the energy, see Figs. 2–3.

The extensivity properties of these expansions are more correct. However, some of the interactions are now multiplicative $(-E_0)$-insertions. It was proven

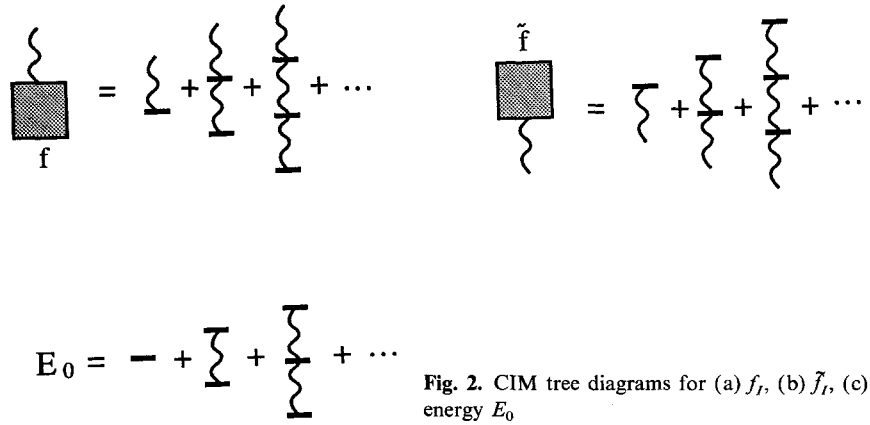

Fig. 2. CIM tree diagrams for (a) f_I, (b) $\tilde{f}_I$, (c) energy E_0

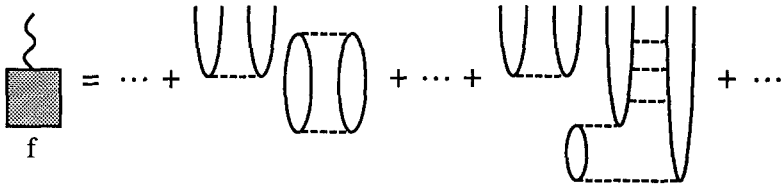

Fig. 3. Disconnected structure of the CIM amplitudes

by Brandow [14] that in the expansion for energy all such diagrams cancel against each other which either contain $(-E_0)$-insertions or are disconnected, provided Pauli exclusion violation is allowed in the remaining fully connected diagrams. This is one form of the celebrated *linked-cluster theorem*, which originally was proven by Goldstone [15] using a different approach. An important fact is nevertheless that the theorem does not help the amplitudes $\tilde{f}, f$ to avoid having disconnected parts (Fig. 3). Indeed, the operators $\tilde{F}$ and F are multiplicatively separable, as concerns their extensivity properties.

3.2. Normal coupled cluster method (NCCM)

The ground-state wave function of a many-body system (or a field theory) can be given in an exponential form [16]:

$$|\Psi\rangle = e^S|0\rangle; \qquad S = \sum_I{}' C_I^\dagger s_I \tag{18}$$

where S is a linked-cluster operator. This was the starting point of the exp S or coupled-cluster method which was developed by Coester and Kümmel [17, 18]. The ground state energy eigenvalue problem can now be given in the form

$$e^{-S}He^S|0\rangle = E_0|0\rangle. \tag{19}$$

The method introduces a *similarity transformation* generated by S, and one of the central features is that the multiple-commutator expansion:

$$e^{-S}He^S = H + [H, S] + \frac{1}{2!}[[H, S], S] + \cdots$$

truncates after a finite number of terms. The amplitudes s_I are solved from the equations:

$$\langle 0|C_I e^{-S}He^S|0\rangle = E_0\delta(I, 0). \tag{20}$$

The structure of these equations almost trivially guarantees the linked-cluster theorem. Not only has the energy a connected expansion, but also the amplitudes s_I will be given exclusively in terms of connected Goldstone diagrams. These features are very important for the correct separability properties in chemistry, and it is not a great surprise that the method was essentially independently introduced into quantum chemistry by Čížek [19] (for reviews see e.g. [20] and the articles in the present volume).

The extensivity properties of the operators F and S are precisely analogous to those of the partition function $Z = \mathrm{Tr}\exp(-H/T)$ and the free energy $F = -T\log Z$ in statistical physics.

In the *normal coupled cluster method* (NCCM) [21, 22] the bra state can also be parametrized as follows:

$$\langle\tilde{\Psi}| = \langle 0|\tilde{S}e^{-S}; \qquad \tilde{S} = 1 + \sum_I{}' \tilde{s}_I C_I. \tag{21}$$

Later it will be seen that S and $\tilde{S}$ are canonically conjugate to each other, and thus $(\tilde{X}, X) = (\tilde{S}, S)$.

Since the normalization is now manifest, i.e. $\langle\tilde{\Psi}|\Psi\rangle = \langle 0|\tilde{S}e^{-S}e^{S}|0\rangle = \tilde{s}_0 = 1$, the variational equations for the energy do not need a Lagrange multiplier. Using the same Hamiltonian as previously, the diagonal energy is:

$$\bar{T} = \langle 0|\tilde{S}e^{-S}Te^{S}|0\rangle = \sum_I{}' \tilde{s}_I T_I s_I, \tag{22}$$

and the stationary equations become:

$$\begin{aligned} \frac{\partial\bar{H}}{\partial\tilde{s}_I} = 0 \Rightarrow s_I &= -\frac{1}{T_I}\frac{\partial\bar{V}}{\partial\tilde{s}_I}, \\ \frac{\partial\bar{H}}{\partial s_I} = 0 \Rightarrow \tilde{s}_I &= -\frac{\eta_I}{T_I}\frac{\partial\bar{V}}{\partial s_I}. \end{aligned} \tag{23}$$

The equations can be iterated to produce diagrammatic expansions for the amplitudes $(\tilde{s}_I, s_I)$.

The average value functional has the ground form:

$$\begin{aligned} \langle H\rangle &= \langle 0|\tilde{S}\{He^{S}\}_{\mathscr{L}}|0\rangle \\ &= \sum_{n=0}^{M}\frac{1}{n!}\sum_I\sum_{J_1}{}'\cdots\sum_{J_n}{}' \tilde{s}_I\langle I|\bar{H}|J_1\cdots J_n\rangle s_{J_n}\cdots s_{J_1}, \end{aligned} \tag{24}$$

where the subscript $\mathscr{L}$ (for "linked") means that every S is linked to H, and the matrix element is:

$$\langle I|\bar{H}|J_1\cdots J_n\rangle = \langle 0|C_I[\cdots[H, C_{J_1}^{\dagger}], \cdots, C_{J_n}^{\dagger}]|0\rangle, \tag{25}$$

and I is allowed also to be the null configuration, whence $\tilde{s}_0 = 1$. As is readily seen, the function is nonlinear in the connected or additively separable amplitudes (s), but linear in the amplitudes $(\tilde{s})$, which turn out to be disconnected and multiplicatively separable.

Figure 4 gives a schematic picture of the average value functional and the matrix element. Iteration of Eq. (23) unravels the structure of the ground-state

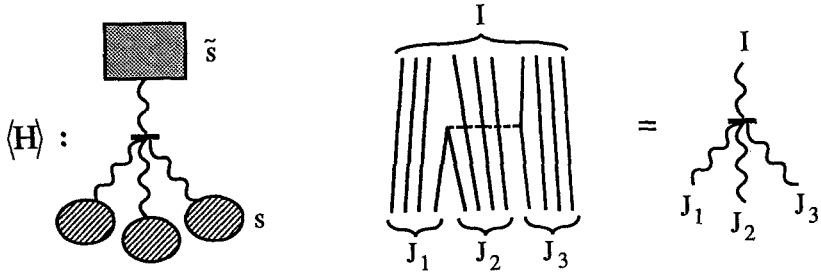

Fig. 4. Schematic representation of the average value functional and a typical matrix element of an operator in NCCM

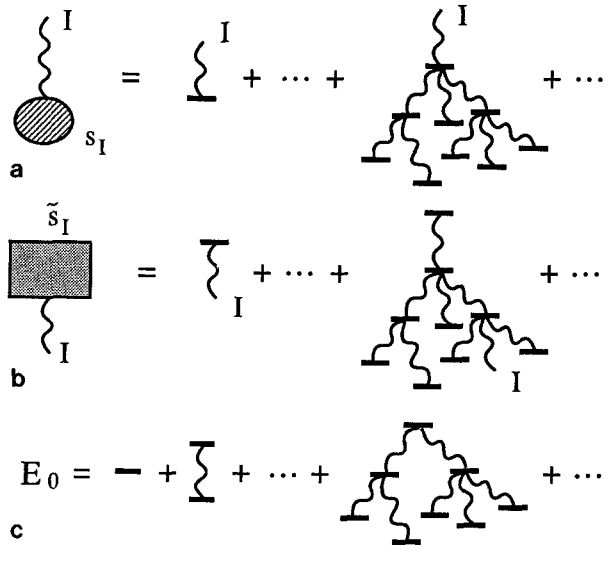

Fig. 5a–c. Diagrammatic NCCM tree structure of **(a)** the connected (additively separable) amplitudes s_I, **(b)** the disconnected (multiplicatively separable) amplitudes $\tilde{s}_I$, and **(c)** the energy. Diagrams for energy are connected, and they have a unique uppermost vertex. In all cases branching occurs only downwards (to the past)

amplitudes $\tilde{s}_I$ and s_I and the energy, displayed also schematically in Fig. 5. Although the *exact* amplitudes $\tilde{s}_I$ are in principle decomposable into multiplicatively separable factors (this feature is not explicitly obvious from the way they are drawn in Fig. 5), the extensivity or separability properties may typically be obscured in approximative calculations.

Both the NCCM and the ECCM are fully consistent with the *Hellmann–Feynman principle* as long as the equations are derived from the variational conditions. Indeed, the introduction of the bra state makes explicit the rather implicit rules derived for the first time within the coupled cluster approach by Monkhorst [23] for the purpose of implementing the Hellmann–Feynman principle. The principle has been applied to practical numerical computations only quite recently (see e.g. by Bartlett et al. [24], whose function Λ is related to the present $\tilde{S}$ by $\tilde{S} = 1 + \Lambda$).

3.3. Extended coupled cluster method (ECCM)

In this method [21] also the bra state is parametrized by additively separable *connected* amplitudes. To be able to do so, one must understand the precise diagrammatic structure of the amplitudes $\tilde{s}_I$. Assuming the exact ket and bra ground states to be known and given in terms of S and $S^\dagger$, it follows by definition that:

$$\langle 0|\tilde{S} = \frac{\langle 0|e^{S^\dagger}e^{S}}{\langle 0|e^{S^\dagger}e^{S}|0\rangle}. \tag{26}$$

A careful consideration of the structure of $\langle 0|e^{S^\dagger}e^{S}$, where both S and $S^\dagger$ are linked-cluster operators, shows that it can be expressed as the product of the multiplicatively separable factor $\langle 0|e^{S^\dagger}e^{S}|0\rangle$, which encompasses all the closed diagrams (and cancels the denominator above), and another multiplicatively separable factor $\langle 0|e^{S''}$, where $S'' \in \mathscr{C}^-$ is a connected annihilation operator. The

average value functional is now:

$$\langle H\rangle = \langle 0|e^{S''}e^{-S}He^{S}|0\rangle. \tag{27}$$

In effect, the method introduces a *double* similarity transformation:

$$\hat{H} = e^{S''}e^{-S}He^{S}e^{-S''}. \tag{28}$$

The ground state eigenvalue equations for the ket and bra states are then:

$$\hat{H}|0\rangle = E_0|0\rangle; \qquad \langle 0|\hat{H} = E_0\langle 0|. \tag{29}$$

Section 6 makes it obvious that in ECCM the canonically conjugate pair of operators are $(\tilde{X}, X) = (\tilde{\Sigma}, \Sigma)$, where:

$$\begin{aligned} \tilde{\Sigma} &\equiv S'' = \sum_I{}' \tilde{\sigma}_I C_I, \\ \Sigma|0\rangle &\equiv Qe^{S''}S|0\rangle; \qquad Q = I^{op} - |0\rangle\langle 0|. \end{aligned} \tag{30}$$

Writing:

$$\Sigma = \sum_I{}' C_I^{\dagger}\sigma_I \tag{31}$$

the connections between s_I and σ_1 are:

$$\begin{aligned} \sigma_I &= \langle 0|C_I e^{S''}S|0\rangle = \langle 0|\tilde{S}C_I S|0\rangle, \\ s_I &= \langle 0|C_I e^{-\tilde{\Sigma}}\Sigma|0\rangle = s_I[\tilde{\sigma}, \sigma]. \end{aligned} \tag{32}$$

It is again straightforward to show that the diagonal part of the Hamiltonian becomes:

$$\bar{T} \equiv \langle 0|e^{S''}e^{-S}Te^{S}|0\rangle = \sum_I{}' \tilde{\sigma}_I T_I \sigma_I. \tag{33}$$

The variational stationary conditions can then be used to derive the equations:

$$\begin{aligned} \frac{\partial \bar{H}}{\partial \tilde{\sigma}_I} = 0 \Rightarrow \sigma_I &= -\frac{1}{T_I}\frac{\partial \bar{V}[\tilde{\sigma}, \sigma]}{\partial \tilde{\sigma}_I}, \\ \frac{\partial \bar{H}}{\partial \sigma_I} = 0 \Rightarrow \tilde{\sigma}_I &= -\frac{\eta_I}{T_I}\frac{\partial \bar{V}[\tilde{\sigma}, \sigma]}{\partial \sigma_I}. \end{aligned} \tag{34}$$

These equations can be solved iteratively to reveal the diagrammatic structure of the amplitudes. The general form of the expectation functional is:

$$\begin{aligned} \langle H\rangle &= \langle 0|\{e^{\tilde{\Sigma}}\{He^{\Sigma}\}_{\mathscr{L}}\}_{\mathscr{D}\mathscr{L}}|0\rangle \\ &= \sum_{m=0}^{\infty}\sum_{n=0}^{M}\frac{1}{m!n!}\sum_{\{I_l\}}{}'\sum_{\{J_l\}}{}'\tilde{\sigma}_{I_1}\cdots\tilde{\sigma}_{I_m}\langle I_1\cdots I_m|\bar{H}|J_1\cdots J_n\rangle\sigma_{J_n}\cdots\sigma_{J_1}. \end{aligned} \tag{35}$$

Here the new subscript $\mathscr{D}\mathscr{L}$ (for "double linking") means that each $\tilde{\Sigma}$ must be linked either to H or, in the absence of such a link, to at least two different Σ. The expression is nonlinear with respect to both $\tilde{\sigma}$ and σ, which are connected, additively separable amplitudes. The double linking property of the average value is proven carefully in Appendix A. An explicit algebraic expression for the matrix element in the bosonic case was derived in [22, Appendix B]. Using the

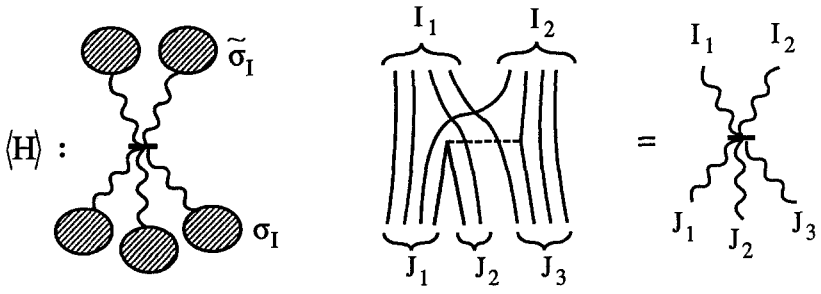

Fig. 6. Schematic illustration of the expectation value functional and the structure of the matrix element in ECCM. There are definite restrictions on how the single-particle lines can be grouped into configurations (see text)

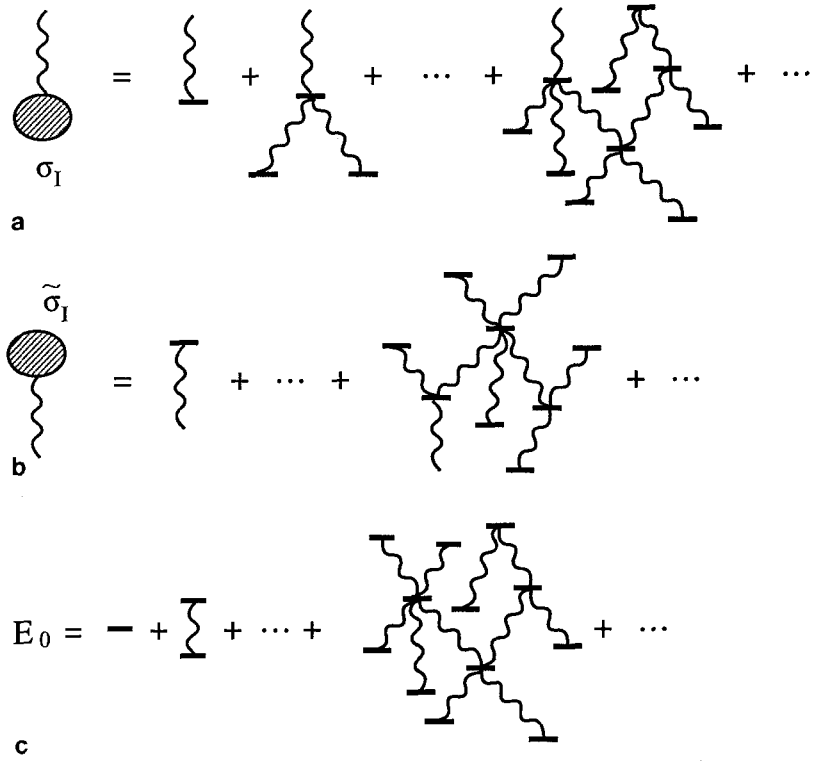

Fig. 7a–c. ECCM tree structure of **(a)**–**(b)** the amplitudes σ_I and $\tilde{\sigma}_I$, **(c)** the energy. All contributions are *connected*. Branching of the trees occurs in both directions

$\mathscr{D}\mathscr{L}$ notation the result is:

$$\langle I_1 \cdots I_m | \bar{H} | J_1 \cdots J_n \rangle = \langle 0 | \{ C_{I_m} \cdots C_{I_1} [\cdots [H, C^\dagger_{J_1}], \cdots, C^\dagger_{J_n}] \}_{\mathscr{D}\mathscr{L}} | 0 \rangle$$
$$= \langle 0 | \{ C_{I_m} \cdots C_{I_1} [H C^\dagger_{J_1} \ldots C^\dagger_{J_n}]_{\mathscr{L}} \}_{\mathscr{D}\mathscr{L}} | 0 \rangle. \quad (36)$$

It is schematically illustrated in Fig. 6 together with the average value of the operator. The iterated *ECCM tree* structures of the amplitudes $(\tilde{\sigma}_I, \sigma_I)$ and the energy are illustrated in Fig. 7. In the present case the tree diagram expansion for the energy is not obvious; it has to be more carefully justified using the topological properties of tree diagrams [21].

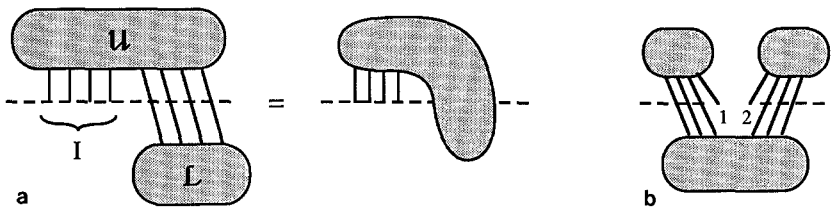

Fig. 8. a Goldstone diagrams summed by $\tilde{\sigma}_I$. Every line $l_j \in I$ is connected to all other $l_k \in I$ via any route within $U + L$. **b** Example of diagrams contributing to $\tilde{\sigma}_2$

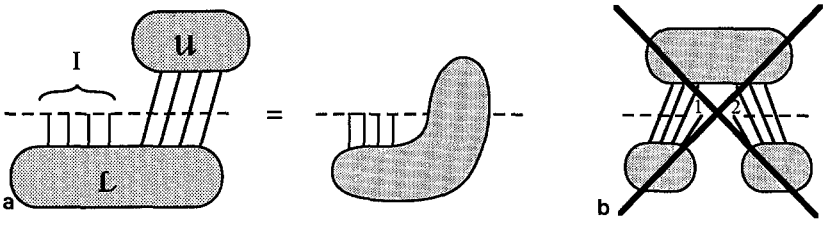

Fig. 9. a Goldstone diagrams for σ_I. Every line $l_j \in I$ is connected to all other $l_k \in I$ through a route *within L*. **b** Example of diagrams *not* contributing to σ_2. Inclusion of this diagram would lead to overcounting

The structure of the average value functional can be alternatively studied by the Bargmann space concepts using the holomorphic wave functionals, in which case a very useful generating functional can be introduced for the expectation values. This approach is briefly discussed in Appendix B.

The amplitudes $\tilde{s}_I$ and $\tilde{\sigma}_I$ have simple physical interpretations. They give the expectation values (connected expectation values, respectively) of the creation operators:

$$\tilde{s}_I = \langle C_I^\dagger \rangle = \langle 0|\tilde{S}C_I^\dagger|0\rangle,$$
$$\tilde{\sigma}_I = \langle C_I^\dagger \rangle_{conn} = \langle 0|\tilde{S}C_I^\dagger|0\rangle_{conn}.$$

Notice that $\sigma_I \neq \langle C_I \rangle_{conn}$. Figures 8–9 give further illumination on the structures of the basic ECCM amplitudes.

In the limit where the Grassmann sources are zero ($\tilde{v} = v = 0$) the odd amplitudes $\tilde{\sigma}_I, \sigma_I (\eta_I = -1)$ may be regarded independent generators of the Grassmann algebra. The other non-connected amplitudes such as $\tilde{f}_I, f_I$ are then higher-order elements of the Grassmann algebra.

4. Technical details

The addition and subtraction of the configuration indices are defined as follows:

$$C_{J-I}^\dagger|0\rangle \equiv C_I C_J^\dagger|0\rangle; \qquad C_{J+I}^\dagger \equiv C_I^\dagger C_J^\dagger, \tag{37}$$
$$\langle 0|C_{I-J} \equiv \langle 0|C_I C_J^\dagger; \qquad C_{I+J} \equiv C_I C_J. \tag{38}$$

Notice that by these definitions the operators C_{I-J}, C_{I+J} etc. are not necessarily normalized. The delta function is likewise generalized:

$$\langle 0|C_I C_J C_K^\dagger|0\rangle = \langle 0|C_{I+J} C_K^\dagger|0\rangle = \delta(I+J, K). \tag{39}$$

Since also $\langle 0|C_I C_J C_K^\dagger|0\rangle = \langle 0|C_I C_{K-J}^\dagger|0\rangle$ by definition, the identity

$$\delta(I+J, K) \equiv \delta(I, K-J) \tag{40}$$

holds. The addition and subtraction can be generalized to several indices. For example, $I_1 \pm I_2 \pm I_3 \pm \cdots \equiv ((I_1 \pm I_2) \pm I_3) \pm \cdots$. The sums are neither commutative nor associative: $I_1 + I_2 - I_3 \neq I_1 + (I_2 - I_3) \neq I_1 - I_3 + I_2$. For the delta function one obtains the chain rule:

$$\delta(I \pm \cdots \pm J, K \pm \cdots \pm L \pm M) = \delta(I \pm \cdots \pm J \mp M, K \pm \cdots \pm L). \tag{41}$$

In precisely the same fashion compound indices are defined for the cluster amplitudes, e.g.:

$$\sigma_{I+J} = \langle 0|C_I C_J \Sigma|0\rangle; \qquad \sigma_{I-J} = \langle 0|C_I C_J^\dagger \Sigma|0\rangle. \tag{42}$$

Clearly $\sigma_{I+J} = \eta_{I,J}\sigma_{J+I}$.

It will be useful to define the matrix functions:

$$\begin{aligned} \omega_{I,J} &\equiv \omega_{J-I} \equiv \langle 0|C_I e^{\Sigma} C_J^\dagger|0\rangle = \langle 0|e^{\Sigma} C_I C_J^\dagger|0\rangle, \\ \bar{\omega}_{I,J} &\equiv \bar{\omega}_{J-I} \equiv \langle 0|C_I e^{-\Sigma} C_J^\dagger|0\rangle = \langle 0|e^{-\Sigma} C_I C_J^\dagger|0\rangle. \end{aligned} \tag{43}$$

These are upper triangular Toeplitz matrices over the configuration index space. They are orthonormal, because:

$$\begin{aligned} \delta(I, J) = \langle 0|C_I C_J^\dagger|0\rangle &= \sum_K \langle 0|C_I e^{\Sigma} C_K^\dagger|0\rangle\langle 0|C_K e^{-\Sigma} C_J^\dagger|0\rangle \\ &= \sum_K \omega_{I,K}\bar{\omega}_{K,J} = \sum_K \omega_{K-I}\bar{\omega}_{J-K}; \end{aligned} \tag{44}$$

likewise is $\sum_K \bar{\omega}_{I,K}\omega_{K,J} = \sum_K \bar{\omega}_{K-I}\omega_{J-K} = \delta(I, J)$. Clearly, rules such as $\omega_{I+J,K} = \omega_{I,K-J} = \omega_{K-J-I} = \omega_{K-(I+J)}$ involving compound indices are also effective.

Partial derivatives of functions of $(\tilde{\sigma}_I, \sigma_I)$ are defined in accordance with:

$$\delta f[\tilde{\sigma}, \sigma] = \sum_I{}' \left(\delta\tilde{\sigma}_I \frac{\partial f}{\partial \tilde{\sigma}_I} + \delta\sigma_I \frac{\partial f}{\partial \sigma_I} \right).$$

Since the average value functional in ECCM is, however, given explicitly in terms of the pair (s'', s), rules must be established for combined derivatives. Thus, for $f[\tilde{\sigma}[s''], \sigma[s'', s]]$:

$$\begin{aligned} \left.\frac{\partial f}{\partial s_I''}\right|_s &= \frac{\partial f}{\partial \tilde{\sigma}_I} + \sum_J{}' \sigma_{I+J} \frac{\partial f}{\partial \sigma_J}, \\ \left.\frac{\partial f}{\partial s_I}\right|_{s''} &= \sum_J{}' \eta_I \eta_{I,J} \omega_{J,I} \frac{\partial f}{\partial \sigma_J}. \end{aligned} \tag{45}$$

It is not possible here to go into great detail; the treatment of the ECCM algebra largely parallels that in [22], but with Grassmann amplitudes allowed.

Among the most important results are the algebraic expressions for various matrix elements of the operators transformed by the double similarity

transformation. For example:

$$\langle 0|C_I\hat{A}|0\rangle \equiv \langle 0|C_I e^{\bar{S}} e^{-S} A e^{S}|0\rangle = (\partial_I \bar{A}) + \sum_J{}' \sigma_{I+J}(\partial_J \bar{A}); \tag{46}$$

$$\langle 0|\hat{A}C_J^\dagger|0\rangle \equiv \langle 0|e^{\bar{S}} e^{-S} A e^{S} e^{-\bar{S}} C_J^\dagger|0\rangle$$

$$= \eta_I \eta_{I,A}(\partial_I \bar{A}) + \eta_{I,A} \sum_J{}' \mathscr{L}_{I,J}(\partial_J \bar{A}) + \eta_{I,A} \sum_J{}' \sum_K{}' \mathscr{L}_{I,J}\sigma_{J+K}(\partial_K \bar{A}). \tag{47}$$

In the latter equation the function $\mathscr{L}$ is:

$$\mathscr{L}_{I,J} \equiv \sum_{KM} \eta_{I,K}\omega_{M+K}\bar{\omega}_{M,I}\bar{\omega}_{K,J} = \langle 0|\{e^{\bar{S}} C_I^\dagger C_J^\dagger\}_{\mathscr{D}\mathscr{L}}|0\rangle. \tag{48}$$

The parities are $\mathscr{L}_{I,J} = \eta_{I,J}\mathscr{L}_{J,I}$ and $\eta_{\mathscr{L}_{I,J}} = \eta_I \eta_J$. The subscript $\mathscr{D}\mathscr{L}$ now denotes restriction to such terms where each $\bar{S}$ is linked to both $C_I^\dagger$ and $C_J^\dagger$. This can be verified by carefully inspecting the algebraic definition of $\mathscr{L}$ [22]. A slightly more complicated expression is obtained for the general matrix element:

$$\langle 0|C_X\hat{A}C_Y^\dagger|0\rangle = \eta_{Y,A}\delta(X, Y)\bar{A} + \eta_X\eta_Y\eta_{Y,A}(\partial_{Y-X}\bar{A}) + \sum_I{}' \eta_{Y,A}\mathscr{L}^X_{Y,I}(\partial_I \bar{A})$$
$$+ \sum_I{}' \sum_J{}' \eta_{Y,A}\mathscr{L}^X_{Y,I}\sigma_{I+J}(\partial_J \bar{A}) + \eta_Y\eta_{Y,A}(\partial_{\bar{X}}\partial_Y \bar{A})$$
$$+ \eta_Y\eta_{Y,A} \sum_I{}' \sigma_{X+I}(\partial_I \partial_Y \bar{A}). \tag{49}$$

Here appears a new function:

$$\mathscr{L}^X_{I,J} \equiv \sum_{K,M} \eta_{I,K}\omega_{X,M+K}\bar{\omega}_{M,I}\bar{\omega}_{K,J} = \langle 0|C_X\{e^{\bar{S}} C_I^\dagger C_J^\dagger\}_{\mathscr{D}\mathscr{L}}|0\rangle, \tag{50}$$

where the double linking requirement obviously does not concern the configuration X of the operator C_X. By using the Wick theorem (to be given below) it is possible to express the functions $\mathscr{L}^X_{I,J}$ in terms of the $\mathscr{L}_{I,J}$:

$$\mathscr{L}^X_{I,J} = \sum_{K,M} \eta_{I,K}\,\delta(X, K+M)\mathscr{L}_{I-M,J-K}.$$

The expectation of product of two operators is easily obtained from:

$$\langle AB\rangle \equiv \langle \tilde{\Psi}|AB|\Psi\rangle = \sum_I \langle 0|\hat{A}C_I^\dagger|0\rangle\langle 0|C_I\hat{B}|0\rangle,$$

upon which point we can use Eqs. (46–47) to derive the result:

$$\langle AB\rangle = \bar{A} * \bar{B} \equiv \bar{A}\bar{B} + \sum_I{}' \sum_J{}' [(\partial_I \bar{A})\chi_{I,J}(\partial_J \bar{B}) + (\partial_I \bar{A})\chi_{I,\bar{J}}(\partial_{\bar{J}}\bar{B})$$
$$+ (\partial_{\bar{I}}\bar{A})\chi_{\bar{I},J}(\partial_J \bar{B}) + (\partial_{\bar{I}}\bar{A})\chi_{\bar{I},\bar{J}}(\partial_{\bar{J}}\bar{B})]. \tag{51}$$

Here the various coefficients are:

$$\chi_{I,J} = \eta_I\eta_{I,A}\left[\sigma_{I+J} + \sum_{K,M}{}' \eta_K\sigma_{I+K}\mathscr{L}_{K,M}\sigma_{M+J}\right],$$

$$\chi_{I,\bar{J}} = \eta_I\eta_{I,A}\left[\delta(I, J) + \sum_K{}' \eta_K\sigma_{I+K}\mathscr{L}_{K,J}\right],$$

$$\chi_{\bar{I},J} = \eta_I\eta_{I,A}\eta_J\eta_{J,B} \sum_K{}' \mathscr{L}_{I,K}\sigma_{K+J}, \tag{52}$$

$$\chi_{\bar{I},\bar{J}} = \eta_I\eta_{I,A}\mathscr{L}_{I,J}.$$

The "star product" introduced above can be applied to products of several factors. It is associative by definition. It should be stressed that all the algebraic expressions discussed in this section also have well understood diagrammatic interpretations.

An important consistency relation can be derived for the average value functional of an operator, on the basis of the specific form of the definition in Eq. (27):

$$\partial_I \tilde{\ast}_J \bar{A} = (\partial_I \partial_J \bar{A}) + \sum_K{}' \sigma_{I+K}(\partial_K \partial_J \bar{A}) + \eta_{I,J} \sum_K{}' \sigma_{J+K}(\partial_K \partial_I \bar{A}) + \sum_K{}' \sum_L{}' \eta_{J,L} \sigma_{I+L} \sigma_{J+K}(\partial_K \partial_L \bar{A}). \tag{53}$$

This identity gives rise to recursion relations between the matrix elements of an operator, similar to those in Ref. [22].

It is often necessary to arrange products of configuration operators into *normal order*. For this purpose an algebraic formulation of the Wick theorem is available:

$$C_I C_J^\dagger = \sum_K Z_K(J, I) C_{J-K}^\dagger C_{I-K}, \tag{54}$$

where

$$Z_K(J, I) = \eta_K \eta_{K,I} \eta_{K,J} \eta_{I,J}. \tag{55}$$

The sign factor Z can be ± 1. For the bosonic algebra this formula was proven in Ref. [22]. The present general form is derived in Appendix C. Equation (54) can be iteratively used also for more complicated operator products.

5. Excited states and transition amplitudes

The average value functional for the energy with its low order (functional) derivatives plays a crucial role in the IC methods in deriving various physical results of interest. As an important example let us consider the excited states of a many-body system. The present treatment is restricted to ECCM and generalizes the results of Ref. [25].

Let the ket and bra eigenvalue equations be written as:

$$\begin{aligned} \hat{H}|\Phi_\lambda\rangle &= (E_0 + \varepsilon_\lambda)|\Phi_\lambda\rangle; \qquad |\Phi_\lambda\rangle \equiv Y^\lambda|0\rangle, \\ \langle\tilde{\Phi}_\lambda|\hat{H} &= (E_0 + \varepsilon_\lambda)\langle\tilde{\Phi}_\lambda|; \qquad \langle\tilde{\Phi}_\lambda| \equiv \langle 0|\tilde{Y}^\lambda, \end{aligned} \tag{56}$$

where $Y^\lambda \in \mathscr{C}^+$ and $\tilde{Y}^\lambda \in \mathscr{C}^-$, and the double similarity transformation is used as defined in Eq. (28). Assume that the exact amplitudes $\tilde{\Sigma}$, Σ for the ground state have been solved. The first functional derivatives of $\bar{H}$ are then zero. Denoting the second functional derivatives of $\bar{H}$ calculated at the ground state by:

$$\begin{aligned} \mathscr{F}_{I,J} &\equiv \eta_I \eta_J \partial_I \partial_J \bar{H}|_{g.s.} = \eta_{I,J} \mathscr{F}_{J,I}, \\ \mathscr{E}_{I,J} &\equiv \eta_J \partial_I \partial_J \bar{H}|_{g.s.}, \\ \tilde{\mathscr{F}}_{I,J} &\equiv \partial_J \partial_I \bar{H}|_{g.s.} = \eta_{I,J} \tilde{\mathscr{F}}_{J,I}, \end{aligned} \tag{57}$$

and using Eq. (49) together with the expansions:

$$\begin{aligned} Y^{\lambda} &= \sum_{I}{}' \, C_I^{\dagger} y_I^{\lambda}, \\ \tilde{Y}^{\lambda} &= \sum_{I}{}' \, \tilde{y}_I^{\lambda} C_I, \end{aligned} \tag{58}$$

the following matrix forms for the eigenvalue equations are obtained:

$$\sum_{J}{}' \left(\mathscr{E}_{I,J} + \sum_{K}{}' \eta_K \sigma_{I+K} \mathscr{F}_{K,J} \right) y_J^{\lambda} = \varepsilon_{\lambda} y_I^{\lambda}, \tag{59}$$

$$\sum_{J}{}' \tilde{y}_J^{\lambda} \left(\mathscr{E}_{J,I} + \sum_{K}{}' \eta_K \sigma_{J+K} \mathscr{F}_{K,I} \right) = \varepsilon_{\lambda} \tilde{y}_I^{\lambda}. \tag{60}$$

Since the Grassmann amplitudes are zero at the ground state, the eigenvalue equations are reducible into independent bosonic and fermionic sectors. The matrix elements above are nonzero only for index combinations *BB* or *FF* corresponding to bosonic and fermionic excitations, respectively, and they are made up of ordinary c-numbers in both cases. In the fermionic case the operators in expansions (58) are odd. The expansion coefficients $\tilde{y}_I^{\lambda}, y_I^{\lambda}$ can always be assumed ordinary numbers, whence the normalization conditions:

$$\langle \tilde{\Phi}_{\lambda} | \Phi_{\lambda'} \rangle = \sum_{I}{}' \, \tilde{y}_I^{\lambda} y_I^{\lambda'} = \delta(\lambda, \lambda') \tag{61}$$

may be imposed. A general ket state, mixing even and odd numbers of fermions, can then be conveniently written as a superposition:

$$|\Phi\rangle = \sum_{\lambda} \phi_{\lambda} Y^{\lambda} |0\rangle,$$

where all terms are Grassmann-even, if the coefficients ϕ_{λ} are Grassmann numbers for those excited states that differ from the model state in fermionic parity.

The results derived in this and the previous section allow also the calculation of the matrix elements of arbitrary operators between the exact eigenstates of the system. These are of particular interest for the evaluation of transition probabilities under external perturbations. Another interesting field which has yet to be more carefully studied is the application of ECCM to the case of degenerate perturbation theory, which is important in atomic and molecular physics. The present formulation lends itself in a natural fashion to the case where the model state is a closed shell system. The particles in an open shell are then added by suitable excitation operators Y^{λ}.

6. Equations of motion

The equations of motion can be derived from the quantum mechanical action functional:

$$\mathscr{A} = \int dt \langle \tilde{\Psi} | (i\partial_t - H) | \Psi \rangle \tag{62}$$

by employing the variational principle independently for the ket and bra states:

$$\begin{aligned} \frac{\delta \mathscr{A}}{\delta \langle \tilde{\Psi}|} = 0 \Rightarrow i\frac{\partial}{\partial t}|\Psi\rangle = H|\Psi\rangle, \\ \frac{\delta \mathscr{A}}{\delta |\Psi\rangle} = 0 \Rightarrow i\frac{\partial}{\partial t}\langle\tilde{\Psi}| = -\langle\tilde{\Psi}|H. \end{aligned} \tag{63}$$

In the various IC parametrizations the functional is always of the form:

$$\mathscr{A} = \int dt \left\{ i \sum_I \tilde{x}_I \dot{x}_I - \bar{H}[\tilde{x}, x] \right\}, \tag{64}$$

where the null term ($I = 0$), however, is excluded in the coupled cluster approaches. For CIM the result is immediately obvious with the replacement $(\tilde{x}_I, x_I) \rightarrow (\tilde{f}_I, f_I)$. In the CC parametrizations the phase or size factors of the Schrödinger wave functions can be dropped since they can be proven to have no effect on the equations of motion for the cluster amplitudes [21, 22]. In NCCM

$$\begin{aligned} \mathscr{A} &= \int dt \langle 0|\tilde{S}e^{-S}(i\partial_t - H)e^{S}|0\rangle \\ &= \int dt \langle 0|\{i\tilde{S}\dot{S} - \bar{H}[\tilde{s}, s]\}|0\rangle = \int dt \left\{ i \sum_I{}' \tilde{s}_I \dot{s}_I - \bar{H}[\tilde{s}, s] \right\}. \end{aligned} \tag{65}$$

This demonstrates that the canonical pair of variables is $(\tilde{X}, X) = (\tilde{S}, S)$.

The derivation is slightly more involved in the case of ECCM. The temporal part of the action can be developed as:

$$\begin{aligned} \mathscr{A}_0 &= i \int dt \langle 0|e^{\tilde{\Sigma}} e^{-S}\, \partial_t e^{S}|0\rangle = i \int dt \langle 0|e^{\tilde{\Sigma}}\dot{S}|0\rangle = -i \int dt \langle 0|\dot{\tilde{\Sigma}} e^{\tilde{\Sigma}} S|0\rangle \\ &= -i \int dt \langle 0|\dot{\tilde{\Sigma}}\Sigma|0\rangle = i \int dt \langle 0|\tilde{\Sigma}\dot{\Sigma}|0\rangle, \end{aligned}$$

from which it is obtained:

$$\mathscr{A} = \int dt \left\{ i \sum_I{}' \tilde{\sigma}_I \dot{\sigma}_I - \bar{H}[\tilde{\sigma}, \sigma] \right\}. \tag{66}$$

Since the canonical variables are now $(\tilde{X}, X) = (\tilde{\Sigma}, \Sigma)$, the expectation functional of the Hamiltonian should be given in terms of these variables instead of the original (S'', S)-amplitudes.

The equations of motion are obtained by requiring stationarity of $\mathscr{A}$ against small variations of the amplitudes. Thus, in all IC methods the cluster amplitudes obey the classical Hamiltonian canonical equations of motion:

$$\begin{aligned} i\dot{x}_I &= \frac{\partial \bar{H}}{\partial \tilde{x}_I} \\ i\dot{\tilde{x}}_I &= -\eta_I \frac{\partial \bar{H}}{\partial x_I}. \end{aligned} \tag{67}$$

Using these equations it is possible to study the temporal behaviour of the expectation value of an arbitrary operator, which may depend explicitly

on time:

$$\frac{d}{dt}\bar{A}[\tilde{x}_I(t), x_I(t), t] = \overline{\frac{\partial A}{\partial t}} + \sum_I{}' \left[\dot{x}_I \frac{\partial \bar{A}}{\partial x_I} + \dot{\tilde{x}}_I \frac{\partial \bar{A}}{\partial \tilde{x}_I} \right]$$
$$= \overline{\frac{\partial A}{\partial t}} - i \sum_I{}' \left[\frac{\partial \bar{H}}{\partial \tilde{x}_I} \frac{\partial \bar{A}}{\partial x_I} - \eta_I \frac{\partial \bar{H}}{\partial x_I} \frac{\partial \bar{A}}{\partial \tilde{x}_I} \right].$$

If the (graded) *Poisson bracket* is defined as:

$$i\{\bar{A}, \bar{B}\} \equiv \sum_I{}' [\eta_I \eta_{I,A} (\partial_I \bar{A})(\partial_{\bar{I}} \bar{B}) - \eta_{I,A} (\partial_{\bar{I}} \bar{A})(\partial_I \bar{B})], \tag{68}$$

the well known classical rule is found (since $\bar{H}$ is Grassmann-even):

$$\frac{d}{dt}\bar{A} = \overline{\frac{\partial A}{\partial t}} + \{\bar{A}, \bar{H}\}. \tag{69}$$

This can be applied also to the canonical variables themselves, whence $\dot{\sigma}_I = \{\sigma_I, \bar{H}\}$; $\dot{\tilde{\sigma}}_I = \{\tilde{\sigma}_I, \bar{H}\}$.

It is also found that the expectation values of the commutators of operators are mapped into Poisson brackets. Using Eqs. (51–52) one gets

$$\langle [A, B] \rangle \equiv \langle \tilde{\Psi} | (AB - \eta_{A,B} BA) | \Psi \rangle = \sum_I{}' [\eta_I \eta_{I,A} (\partial_I \bar{A})(\partial_{\bar{I}} \bar{B}) - \eta_I \eta_{I,B} \eta_{A,B} (\partial_I \bar{B})(\partial_{\bar{I}} \bar{A})],$$

which is transcribed into the result:

$$\langle [A, B] \rangle = i\{\bar{A}, \bar{B}\}. \tag{70}$$

The Poisson bracket and many other expressions would obtain a simpler form by introducing the *right* derivatives $\vec{\partial}_I$ which remove a factor from the right end of a product, in addition to the conventional left derivatives $\partial_{\bar{I}} \equiv \vec{\partial}_{\bar{I}}$. Using this notation:

$$i\{\bar{A}, \bar{B}\} = \sum_I{}' [(\vec{\partial}_I \bar{A})(\vec{\partial}_{\bar{I}} \bar{B}) - \eta_{A,B} (\vec{\partial}_I \bar{B})(\vec{\partial}_{\bar{I}} \bar{A})]. \tag{71}$$

7. Small oscillations and normal modes

The limit of small oscillations around a stationary point reveals the eigenenergies and eigenfrequencies of the system, and allows to calcuate the dynamical linear response to small external perturbations. It is sufficient to expend the Hamiltonian up to second order around the stationary point:

$$\bar{H} = E_0 + \sum_{IJ}{}' \{ \tfrac{1}{2} \delta\tilde{\sigma}_I \delta\tilde{\sigma}_J \mathscr{F}_{I,J} + \tfrac{1}{2} \mathscr{F}_{I,J} \delta\sigma_J \delta\sigma_I + \delta\tilde{\sigma}_I \mathscr{E}_{I,J} \delta\sigma_J \} + \cdots, \tag{72}$$

where the coefficients are as defined in Eq. (57). The equations of motion linearize and can be given in the following block matrix form:

$$i \frac{d}{dt} \begin{bmatrix} \delta\sigma_I \\ \delta\tilde{\sigma}_I \end{bmatrix} = \sum_J{}' \mathscr{H}_{I,J} \begin{bmatrix} \delta\sigma_J \\ \delta\tilde{\sigma}_J \end{bmatrix}, \tag{73}$$

where the *dynamical matrix* is:

$$\mathscr{H}_{I,J} = \begin{bmatrix} \mathscr{E}_{I,J} & \eta_J \tilde{\mathscr{F}}_{J,I} \\ -\mathscr{F}_{I,J} & -\eta_J \eta_{I,J} \mathscr{E}_{J,I} \end{bmatrix}. \tag{74}$$

At the ground state all Grassmann amplitudes are zero. Since the Hamiltonian is Grassmann-even by definition, the entries in the matrix are zero if the indices I, J are of opposite Grassmann parity. Therefore the calculation again reduces into independent bosonic and fermionic sectors. In the bosonic case:

$$\mathscr{H}^B = \begin{bmatrix} \mathscr{E} & \tilde{\mathscr{F}} \\ -\mathscr{F} & -\mathscr{E}^T \end{bmatrix} = \begin{bmatrix} 0 & I \\ -I & 0 \end{bmatrix} \cdot \begin{bmatrix} \mathscr{F} & \mathscr{E}^T \\ \mathscr{E} & \tilde{\mathscr{F}} \end{bmatrix}, \tag{75}$$

where superscript T denotes the transpose of a matrix. In the fermionic sector:

$$\mathscr{H}^F = \begin{bmatrix} \mathscr{E} & -\tilde{\mathscr{F}}^T \\ -\mathscr{F} & -\mathscr{E}^T \end{bmatrix} = \begin{bmatrix} 0 & I \\ I & 0 \end{bmatrix} \cdot \begin{bmatrix} -\mathscr{F} & -\mathscr{E}^T \\ \mathscr{E} & -\tilde{\mathscr{F}}^T \end{bmatrix}. \tag{76}$$

Notice that the matrices $\mathscr{F}$ and $\tilde{\mathscr{F}}$ are *symmetric* in the bosonic case and *antisymmetric* in the fermionic case. Therefore the dynamical matrix is always a product of a symmetric matrix with an antisymmetric one. The characteristic polynomial $\det(\mathscr{H} - \varepsilon I)$ is then a function of ε^2, and the eigenfrequencies appear in pairs

$$\varepsilon = \pm \varepsilon_\lambda. \tag{77}$$

The ε_λ are the excitation energies:

$$\varepsilon_\lambda = E_\lambda - E_0.$$

Let the *positive-frequency* and *negative-frequency* solutions be:

$$\begin{bmatrix} \varphi_I(\varepsilon_\lambda) \\ \chi_I(\varepsilon_\lambda) \end{bmatrix}, \quad \begin{bmatrix} \varphi_I(-\varepsilon_\lambda) \\ \chi_I(-\varepsilon_\lambda) \end{bmatrix},$$

respectively. These are all linearly independent. Their normalization can be chosen as follows:

$$\sum_I{}' [\chi_I(-\varepsilon)\varphi_I(\varepsilon') \mp \varphi_I(-\varepsilon)\chi_I(\varepsilon')] = \begin{cases} \delta(\varepsilon, \varepsilon')\ \mathrm{sgn}(\varepsilon) \\ \delta(\varepsilon, \varepsilon') \end{cases}. \tag{78}$$

Above, upper and lower choices correspond to bosons and fermions, respectively, and $\varepsilon, \varepsilon'$ can be any of $\pm\varepsilon_\lambda$.

Small oscillations are diagonalized into *normal modes* by the expansion:

$$\begin{bmatrix} \delta\sigma_I \\ \delta\tilde{\sigma}_I \end{bmatrix} = \sum_\lambda \psi_\lambda \begin{bmatrix} \varphi_I(\varepsilon_\lambda) \\ \chi_I(\varepsilon_\lambda) \end{bmatrix} + \sum_\lambda \tilde{\psi}_\lambda \begin{bmatrix} \varphi_I(-\varepsilon_\lambda) \\ \chi_I(-\varepsilon_\lambda) \end{bmatrix}. \tag{79}$$

The eigenvectors are composed of ordinary c-numbers. The amplitudes $\psi, \tilde{\psi}$ of the normal modes are c-numbers for bosonic, and Grassmann numbers for fermionic modes. If the above decomposition is inserted into the expansion of Eq. (72) of the Hamiltonian, and orthogonality relations are taken into account, the Hamiltonian becomes diagonalized and is, up to second order terms:

$$\bar{H} = E_0 + \sum_\lambda \varepsilon_\lambda \tilde{\psi}_\lambda \psi_\lambda + \cdots. \tag{80}$$

The transformation into normal coordinates is canonical, and it leaves invariant the form of the equations of motion:

$$i\frac{d}{dt}\psi_\lambda = \frac{\partial \bar{H}}{\partial \tilde{\psi}_\lambda},$$
$$i\frac{d}{dt}\tilde{\psi}_\lambda = -\eta_\lambda \frac{\partial \bar{H}}{\partial \psi_\lambda}. \tag{81}$$

All the various IC methods can be treated in the same fashion. They differ typically from each other, because in CIM both the coefficients $\mathscr{F}$ and $\tilde{\mathscr{F}}$ are zero, and in NCCM $\tilde{\mathscr{F}}$ are zero. Thus, in CIM the dynamical matrix is block diagonal, and it follows that $\chi_I(\varepsilon_\lambda) = \varphi_I(-\varepsilon_\lambda) = 0$. The small oscillations are then:

$$\delta f_I(t) = \sum_\lambda \psi_\lambda(t)\varphi_I(\varepsilon_\lambda),$$
$$\delta \tilde{f}_I(t) = \sum_\lambda \tilde{\psi}_\lambda(t)\chi_I(-\varepsilon_\lambda).$$

There appears no mixing of the positive and negative frequency solutions.

In NCCM the dynamical matrix is lower triangular, and from the eigenvectors the components $\varphi_I(-\varepsilon_\lambda)$ are zero. Thus:

$$\delta s_I(t) = \sum_\lambda \psi_\lambda(t)\varphi_I(\varepsilon_\lambda),$$
$$\delta \tilde{s}_I(t) = \sum_\lambda \psi_\lambda(t)\chi_I(\varepsilon_\lambda) + \sum_\lambda \tilde{\psi}_\lambda(t)\chi_I(-\varepsilon_\lambda).$$

Only the basic amplitudes $\tilde{s}_I$ mix positive and negative frequencies. The ECCM is a general case, where mixing of the positive and negative frequencies appear in both canonical amplitudes $\tilde{\sigma}_I$, σ_I. We can understand the growing mixing in the coupled cluster methods by observing that an increasing number of the basic amplitudes are defined mixtures of both the ket and the bra state parametrizations ($\tilde{S}$ in NCCM and $\tilde{\Sigma}$, Σ in ECCM).

Let the coupled cluster amplitudes σ_I, $\tilde{\sigma}_I$ be given in terms of the normal coordinates as determined around the stationary point in the ECCM phase space:

$$\sigma_I = \sigma_I^0 + \sum_\lambda [\psi_\lambda \varphi_I(\varepsilon_\lambda) + \tilde{\psi}_\lambda \varphi_I(-\varepsilon_\lambda)],$$
$$\tilde{\sigma}_I = \tilde{\sigma}_I^0 + \sum_\lambda [\psi_\lambda \chi_I(\varepsilon_\lambda) + \tilde{\psi}_\lambda \chi_I(-\varepsilon_\lambda)]. \tag{82}$$

If these are inserted into the Hamiltonian without truncating after second order, one obtains the expansion:

$$\bar{H} = E_0 + \sum_\lambda \varepsilon_\lambda \tilde{\psi}_\lambda \psi_\lambda + \frac{1}{3!}\sum_{\lambda\lambda'\lambda''} \tilde{\psi}_\lambda \tilde{\psi}_{\lambda'} \tilde{\psi}_{\lambda''} \langle \lambda\lambda'\lambda'' | \bar{H} | \rangle + \frac{1}{2!}\sum_{\lambda\lambda'\mu} \tilde{\psi}_\lambda \tilde{\psi}_{\lambda'} \langle \lambda\lambda' | \bar{H} | \mu \rangle \psi_\mu$$
$$+ \frac{1}{2!}\sum_{\lambda\mu\mu'} \tilde{\psi}_\lambda \langle \lambda | \bar{H} | \mu\mu' \rangle \psi_{\mu'} \psi_\mu + \frac{1}{3!}\sum_{\mu\mu'\mu''} \langle | \bar{H} | \mu\mu'\mu'' \rangle \psi_{\mu''} \psi_{\mu'} \psi_\mu + \cdots. \tag{83}$$

The higher-order terms describe nonlinear interactions between the normal modes. In an accompanying paper [26] this expansion is explicitly constructed for a simple field theoretical model. Just as the amplitudes σ, $\tilde{\sigma}$ present an

additively separable quasilocal parametrization of the ECCM phase space, one can expect the normal coordinates $\psi, \tilde{\psi}$ to have qualitatively similar properties, assuming the diagonalization can be made. In fact this is not at all an innocent statement. The states λ should also incorporate the totality of nonlocal multiple excitations which are nevertheless expected almost always to effectively dynamically decouple from the more ordinary states, except rarely when their distant parts remain coherent like in an EPR experiment. It should also be emphasized that the stationary conditions may produce states that are topologically distorted in comparison with the ground state or other stationary solutions. The quasilocal parametrization which is a particular generalization of the mean field theory is expected to be able to describe such phenomena. The ECCM parametrization can be interpreted to perform a mapping of the *global* concepts of the state in a Hilbert space with its *linear dynamics* into a *quasilocal* phase space description in terms of additively separable coordinates obeying *nonlinear dynamics*.

8. Bugs?

In truncations of relatively low order the coupled cluster methods are reasonably straightforward to apply, and they yield results that are typically among the best in comparison with any other methods. Proceeding to truncation levels of higher order (e.g. in the SUB N hierarchy) becomes rapidly tedious due to the multivariate nature of the basic variables and increasing complexity of the equations. An important motivation for attempting to do so is the hope that the results might systematically indefinitely improve. Some attempts to numerically test convergence in very high orders in NCCM have been made with the anharmonic oscillator [27, 28], but the results were not fully decisive. Similar computations using ECCM have so far suffered from even greater numerical difficulties preventing firm conclusions [29], although it is more probable than not that there is no such convergence. It thus seems that the convergence properties of the CC methods in high order truncations are not yet sufficiently well understood. Another and even more interesting is the question of the behaviour of the *exact* CC amplitudes for various physical problems. In the following discussion only a few of these problems are considered.

The additively separable linked cluster operators, such as S or $\tilde{\Sigma}$, are mathematically complicated objects. For example, in the case of anharmonic oscillators the operator S is unbounded and its domain is empty, $D(S) = \{\psi \in \mathscr{H} : \|S\psi\| < \infty\} = \varnothing$. It has been pointed out [30, 11] that such operators nevertheless have well defined meaning which can be explored using the holomorphic representations of the wave functions in the Bargmann Hilbert space. In the same context it is easy to show that the Hilbert space contains states for which the operators $\tilde{S}$ or $\tilde{\Sigma}$ cannot be defined, even though they can be defined on a dense subset of states. Furthermore, the operator Σ turns out to be even more problematic, because its series expansion in terms of $\tilde{s}_I$ and s_I diverges. Analogous divergent expansions are obtained for expectation values of many operators, like e.g. for the operator $a^\dagger a$, both in NCCM and ECCM. All such summations can however be regularized by the Bargmann space methods; the divergencies typically result from incorrect formal expansions of exact convergent integrals.

The approach of using the holomorphic wave functions is described more thoroughly elsewhere [11, 26]. Since the approach is of great importance for the

regularization of the coupled cluster methods, Appendix B considers the holomorphic representation and introduces the generating functional for the expectation values for the general case of a mixture of bosons and fermions. The formalism is also applicable to field theories.

Practical applications to realistic physical systems pose much more difficult problems. In the conventional coupled cluster methods a lot of practical wisdom exists concerning truncations, basis sets and other details in various applications, as demonstrated by the many articles in the present volume. The ECCM is largely short of comparable experience, although a considerable amount of analytical and numerical work has been done. One of the basic practical problems is the shortage of universal case-independent trunction schemes capable of ensuring reasonable solutions.

In approximations of increasing truncation order the number of terms or diagrams to be incorporated grows rapidly. Therefore it would be very useful to have suitable symbolic programs which automatically can perform the necessary algebraic manipulations. For this purpose it is important to express the algebraic structure of the theory in a transparent and logical form. Indeed, this is one of the goals of the present paper. In a sense the algebraically formulated CC methods "solve" the diagram classification problem which in other methods necessarily leads to complicated considerations of the topological properties of the Feynman or Goldstone diagrams.

9. Mappings

The IC methods transform the mathematical structure into quantum mechanical the structure of classical mechanics. They also perform a definite "bosonization" or "fermionization" of the quantum mechanical system, i.e. a mapping of the Hilbert space $\mathscr{H}$ into a larger space $\mathscr{B}^{\mathscr{H}}$ together with a suitable mapping of the operator algebras. Conventionally boson expansion methods are used for fermionic systems for example in order to be able to describe their low-lying collective excited states as classical excitations using the coherent states of the bosonized Hilbert space. The original Hilbert space is typically mapped onto a subspace of the bosonized larger space, and the physical subspace is invariant under the bosonized image of the operator algebra (for review, see e.g. [31]). The new structure is again that of quantum mechanics, but with superfluous degrees of freedom related to the nonphysical complement in the large space.

In the IC methods the boson expansion method (supplemented with fermion expansion) is in a sense carried to the logical conclusion with the result that the emerging framework is classical mechanics instead of another form of quantum theory. The discussion below is restricted to ECCM, although part of it applies to the other IC cases as well. Corresponding to the configuration indices of the Hilbert space $\mathscr{H}$ one can define ideal canonical operators $I \mapsto \alpha_I, \alpha_I^\dagger$ obeying the standard commutation relations:

$$\begin{aligned} &[\alpha_I, \alpha_J] \equiv \alpha_I \alpha_J - \eta_{I,J} \alpha_J \alpha_I = [\alpha_I^\dagger, \alpha_J^\dagger] = 0, \\ &[\alpha_I, \alpha_J^\dagger] = \delta(I, J). \end{aligned} \tag{84}$$

An orthonormal basis in $\mathscr{B}^{\mathscr{H}}$ is provided by the states:

$$\prod_{I\rightarrow} \left(\frac{1}{\sqrt{m_I!}} \alpha_I^{\dagger m_I} \right) |0), \tag{85}$$

where $|0)$ is a cyclic state with the property $\alpha_I|0) = 0, \forall I$, and m_I are $\{0, 1\}$ or $\{0, 1, 2, \ldots\}$ depending whether I is a fermionic or bosonic configuration index.

Let the generators of the (bi)coherent states of $\mathscr{B}^{\mathscr{H}}$ be:

$$G_c = G_c[\tilde{\sigma}_I, \sigma_I] = \sum_I{}' (\alpha_I^\dagger \sigma_I - \tilde{\sigma}_I \alpha_I).$$

Then:

$$\begin{aligned} \alpha_I e^{G_c}|0) &= \sigma_I e^{G_c}|0), \\ (0|e^{-G_c}\alpha_I^\dagger &= (0|e^{-G_c}\tilde{\sigma}_I. \end{aligned} \tag{86}$$

These bicoherent states can equivalently be expressed in the ECCM SUB 1 form using $S_c = \sum_I' \alpha_I^\dagger \sigma_I$, $S_c'' = \sum_I' \tilde{\sigma}_I \alpha_I$. Let it be required that the "boson image" O^B of an arbitrary operator O satisfies the identity

$$(0|e^{-G_c}O^B e^{G_c}|0) = \bar{O}[\tilde{\sigma}_I, \sigma_I] \equiv \langle 0|e^{\tilde{S}}e^{-S}Oe^{S}|0\rangle.$$

This is accomplished by choosing:

$$\begin{aligned} O^B[\alpha_I^\dagger, \alpha_I] &= :O^B[\alpha_I^\dagger, \alpha_I]: \\ &= \sum_{m,n} \frac{1}{m!n!} \sum_{\{I_l\}}{}' \sum_{\{J_l\}}{}' \alpha_{I_1}^\dagger \cdots \alpha_{I_m}^\dagger \langle I_1 \cdots I_m|\bar{O}|J_1 \cdots J_n\rangle \alpha_{J_n} \cdots \alpha_{J_1}, \end{aligned} \tag{87}$$

where the matrix elements are as defined in Sect. 3.3; hence $O^B[\tilde{\sigma}_I, \sigma_I] \equiv \bar{O}[\tilde{\sigma}_I, \sigma_I]$. The boson image of an operator is thus obtained by naively canonically quantizing its average value expression. The action functional can also be expressed in the mapped form using the bicoherent states of $\mathscr{B}^{\mathscr{H}}$.

Taking into account the above construction a physical state can thus be represented in a number of equivalent ways:

(a) a binormalized pair of states $\langle\tilde{\Psi}|$ and $|\Psi\rangle$, both of finite norm and with the restrictions $\langle\tilde{\Psi}|\Psi\rangle = 1$, $\tilde{\Psi} \propto \Psi$, in the spaces $(\mathscr{H}^*, \mathscr{H})$, where $\mathscr{H}^*$ is the dual of $\mathscr{H}$, i.e. the space of linear functionals on $\mathscr{H}$,

(b) a bicoherent state in $\mathscr{B}^{\mathscr{H}}$ and its dual,

(c) a point $P = (\tilde{\sigma}, \sigma)$ in the ECCM phase space $\Gamma^{\mathscr{H}}$.

This can be stated in a slightly unprecise but transparent form as

$$\mathscr{H} \sim coh(\mathscr{B}^{\mathscr{H}}) \sim scoh(\mathscr{H}) \equiv \Gamma^{\mathscr{H}}, \tag{88}$$

where $scoh(\mathscr{H})$ is the *supercoherent map* of $\mathscr{H}$ and defined as synonymous to the classical phase space $\Gamma^{\mathscr{H}}$. Obviously the physical states correspond only to a submanifold in the space spanned by all possible values of the coordinates $P = (\tilde{\sigma}, \sigma)$.

The IC treatment of the many-body problem introduces a *supercoherent bosonization* and *fermionization*; in the present context the terminology does not refer merely to fermionic coherent states or to supersymmetry. Instead, while the bosonic and fermionic coherent states of a Hilbert space are used to define a semiclassical *approximation* for the system, the supercoherent states provide an *exact* and completely classicized description. Of the various IC methods only ECCM fully preserves the nonlinearity of the Hamiltonian (albeit at the loss of formal hermiticity in the original coordinate system). This is intimately connected with the fact that all phase space coordinates in the classicized description are additively separable.

Irrespective of the topological properties of the index space $\mathscr{I}$, which may for example be discrete, the spaces above can be considered differentiable manifolds. Without a detailed study it is however not obvious whether in each case the mappings between the various representations are diffeomorphisms or even homeomorphisms. On the contrary, because of the rather singular nature of the CC parametrizations, the correspondence between $\mathscr{H}$ as a manifold and $scoh(\mathscr{H})$ may generally be topologically very complicated. It is also clear that the CC classical map of a quantum theory does not precisely correspond to conventional classical mechanics in spite of the fact that both are based on the concepts of phase space, Hamiltonian and flow. Studies of simple examples (e.g. anharmonic oscillators, double well oscillators, and other simplified $(0+1)$-dimensional field theory models) also show that the representation of a physical state in $\Gamma^{\mathscr{H}}$ is not always unique; i.e. different points in the phase space may represent the same state, and temporal development may sometimes require discontinuous jumps from one coordinate atlas to another, instead of smooth change. These peculiar features (which are probably highly overemphasized in the zero dimensional field theories mentioned above) have yet to be thoroughly understood.

10. Concluding remarks

The methods discussed in this paper treat a problem where the Hamiltonian and the Hilbert space are assumed to be known in advance, and perform a dequantization, i.e. a mapping into an equivalent classical formalism. A natural additional ingredient to the present subject is a discussion of the quantization of an originally classical problem. As a result we are in the position of describing the whole cycle of transformations from one classical Hamiltonian formalism back into another such formalism. The fact that the forms of the Hamiltonians are potentially qualitatively similar in the ECCM case is exciting and raises interesting expectations.

A system in classical mechanics is specified by the phase space Γ and the Hamiltonian H, which determines the flow in the phase space. The cycle of transformations is symbolically

$$(\Gamma, H) \xrightarrow{\mathscr{Q}} (\mathscr{H}, H^{op}) \xrightarrow{\mathscr{CM}} (\Gamma', H'), \tag{89}$$

where $\mathscr{Q}$ denotes quantization and $\mathscr{CM}$ dequantization, or the classical mapping in terms of additively separable phase space coordinates. The new classical phase space and the Hamiltonian are functions of the original ones:

$$\begin{cases} \Gamma' = f_\Gamma(\Gamma, H) \\ H' = f_H(\Gamma, H). \end{cases} \tag{90}$$

Here the functions f_Γ, f_H are in principle known. In simple cases like anharmonic oscillators the mappings can be understood and constructed in detail (see e.g. [11, 26]). Typically (Γ', H') are much more complicated than the original (Γ, H). For example, the number of phase space dimensions may drastically increase.

If the mapped system is integrable, there exist invariant submanifolds in Γ' of lower dimensionality within which the trajectories are confined. A trivial example is the system of harmonic oscillators, or a system diagonalizable by a Bogoliubov transformation, in which cases there exists a submanifold isomorphic to Γ. Even if isolating integrals of motion do not exist, the dynamics in Γ' is very

probably highly nonergodic, and there occurs an effective compactification of the phase space. This is suggested by several clues, e.g. by the fact that the number of independent degrees of freedom in the thermodynamical sense does not essentially increase on quantization; the counterassumption of ergodicity would lead to a specific heat which is proportional to the number of coordinate dimensions in the phase space. As a matter of fact, since quantum mechanics is a linear theory, quantization of a classical system makes the mapped H' formally always integrable; this is evidenced by the quadratic form of the CI energy functional. Some of this integrability and associated compactification may remain also in the CC descriptions. For example, if the original theory is a continuous field theory, e.g. a fiber bundle where the base space is a finite-dimensional manifold, the resulting mapped theory has the capability of being another fiber bundle, although with a more complicated fiber. This is a consequence of the additive separability of the ECCM coordinate system, which allows the linked-cluster many-particle amplitudes to be given as functions of only one position and a set of internal degrees of freedom which must be intricately restricted due to the couplings with other cluster amplitudes and overall normalizability of the many-body wave function.

The previous discussion suggests that it may be possible to find nontrivial systems which are *fixed points* of the transformation and satisfy

$$\begin{cases} \Gamma^* \sim f_\Gamma(\Gamma^*, H^*) \\ H^* \sim f_H(\Gamma^*, H^*), \end{cases} \tag{91}$$

either literally or in the sense of invariant submanifolds. The conditions can be stated also in a compact form by requiring the identity

$$H[\varphi] \sim H[\,*\,\varphi], \tag{92}$$

where $H[\varphi]$ is the original Hamiltonian, φ designates the set $(\tilde{\sigma}, \sigma)$ of canonical coordinates, and $H[\,*\,\varphi]$ is the quantized Hamiltonian, obtained from H by replacing all products of φ by the star products as defined by Eq. (51). The suggested isomorphy between the classical and the quantized phase space raises deep topological problems with regard to the structure of the index space $\mathscr{I}$ and its transforms under canonical transformations.

The possible solution corresponds to a system which suffers no change under quantization. A fixed point, or a self-quantized system, if it existed, would be a very special system. Calculation of its properties could be done using at will either classical mechanics or quantum mechanics. In the latter case, diagram expansions (Feynman, Goldstone) in perturbation theory are exact already at the tree level. The structure of the phase (or Hilbert) space would guarantee that all such diagrams cancel against each other that have loops. If the solution is a fiber bundle theory, it must be free of gauge anomalies, and the symmetries of the classical field theory are carried unchanged to the quantized case. This is clear because the contributions to anomalies from loops must precisely cancel. Indeed, the present coupled cluster approach may offer useful construction principles for such particular anomaly-free theories.

In conclusion, while the principal motivation underlying the study of the coupled cluster methods has been in developing practical approximation hierarchies intended for computations of high accuracy, the present paper suggests that very exciting possibilities may exist for their application into problems of fundamental kind.

Appendix A. Proof of the double-linking structure of the ECCM expectation functional

The starting point is the NCCM representation for the average value as given in Eqs. (24–25). If the amplitudes s_I are expressed in terms of the ECCM amplitudes, using Eqs. (32),

$$s_I = \sum_J{}' \bar{\omega}_{I,J}\sigma_J,$$

the average value is cast into the form

$$\langle O\rangle = \sum_n \frac{1}{n!}\sum_{\{J\}}{}' \sum_{\{K\}} \langle 0|e^{\tilde{\Sigma}}[\cdots[O, C^\dagger_{K_1}], \cdots, C^\dagger_{K_n}]|0\rangle$$
$$\times (\bar{\omega}_{K_n,J_n}\sigma_{J_n})\cdots(\bar{\omega}_{K_1,J_1}\sigma_{J_1}). \tag{A1}$$

Consider first the summation with respect to K_n. Introducing the abbreviation

$$R = [\cdots[O, C^\dagger_{K_1}], \cdots, C^\dagger_{K_{n-1}}]$$

and letting for simplicity the dummy index be $K_n = L$ one obtains

$$\mathrm{Sum}_n \equiv \sum_L \langle 0|e^{\tilde{\Sigma}}[R, C^\dagger_L]|0\rangle\bar{\omega}_{L,J_n} = \sum_L \langle 0|e^{\tilde{\Sigma}}RC^\dagger_L|0\rangle\langle 0|C_L e^{-\tilde{\Sigma}}C^\dagger_{J_n}|0\rangle$$
$$-\sum_L \eta_{L,O}\prod_{j=1}^{n-1}\eta_{L,K_j}\cdot\langle 0|e^{\tilde{\Sigma}}C^\dagger_L R|0\rangle\langle 0|C_L e^{-\tilde{\Sigma}}C^\dagger_{J_n}|0\rangle. \tag{A2}$$

Let the following notation be introduced:

$$R' = R - \sum_L C^\dagger_L\langle 0|C_L R|0\rangle.$$

It is readily found that if $R = \sum_I \sum_J r_{I,J}C^\dagger_I C_J$, then $R' = \sum_I \sum_J{}' r_{I,J}C^\dagger_I C_J$. That is, R' is otherwise the same as R, but the purely creative operator terms are ignored. Thus, the operator R' must contain absorption in all its terms, and, for example, $R'|0\rangle = 0$. Using this notation and the closure in the first term of Eq. (A2), and inserting the resolution of identity between $C^\dagger_L$ and R in the second term, one finds

$$\begin{aligned}\mathrm{Sum}_n &= \langle 0|e^{\tilde{\Sigma}}R'e^{-\tilde{\Sigma}}C^\dagger_{J_n}|0\rangle \\ &= \langle 0|\{e^{\tilde{\Sigma}}R'\}_{\mathscr{L}}C^\dagger_{J_n}|0\rangle.\end{aligned} \tag{A3}$$

Here the subscript $\mathscr{L}$ means in the usual NCCM sense that each $\tilde{\Sigma}$ in the exponent must be linked to the operator R'.

From this equation the following conclusions naturally emerge:

1. From σ_{J_n} at least one line is connected directly to the operator O. *Proof*: Since R' comprises of those terms of $[\cdots[O, C^\dagger_{K_1}], \cdots, C^\dagger_{K_{n-1}}]$ that contain at least one annihilation operator, and the annihilation operators can originate only from O, the statement is obvious.

2. Each line of σ_{J_n} is connected

2.1. either to the operator O (obvious possibility, see above)

2.2. or, if not, to such an operator $\tilde{\Sigma}$ from which there must be a connection

2.2.1. either to the operator O

2.2.2. or, if not, to at least one other amplitude σ_{J_l}.

Proof of 2.2: The last line of Eq. (A3) shows that if a line from $C^\dagger_{J_n}$ is not absorbed by R', it must be absorbed by a $\tilde{\Sigma}$ from which a connection descends to R'. This connection goes either into O (which corresponds to case 2.2.1) or into one of the operators $C^\dagger_{K_l}$, $l = 1, \ldots, n-1$. In the latter case the connection propagates eventually into a σ_{J_l}, because each $K_l \subset J_l$, if $\bar{\omega}_{K_L,J_l} \neq 0$. This completes the proof.

Because Eq. (A1) is symmetric with respect to permutations of $\{\sigma_{J_l}\}$ with appropriate sign factors, the above construction can be repeated for every index J_l. One of the conclusions is that any term where a line from σ_{J_l} is swallowed by the factor $\exp(-\tilde{\Sigma})$ in $\bar{\omega}_{K_l,J_l}$ is cancelled against other similar contraction terms, leaving only such terms where *all* lines of the $\{\sigma_{J_l}\}$ propagate into either O or the factor $e^{\tilde{\Sigma}}$ in front of Eq. (A1). The ECCM matrix element

$$\langle I_1 \cdots I_m | \bar{O} | J_1 \cdots J_n \rangle$$

$$= \sum_{\{K_l\}} \langle 0 | C_{I_m} \cdots C_{I_1} [\cdots [O, C^\dagger_{K_1}], \cdots, C^\dagger_{K_n}] | 0 \rangle \bar{\omega}_{K_n,J_n} \ldots \bar{\omega}_{K_1,J_1}$$

$$\cdot (\eta_{J_2,J_1}\eta_{J_2,K_1})(\eta_{J_3,J_2}\eta_{J_3,J_1}\eta_{J_3,K_2}\eta_{J_3,K_1}) \cdots (\eta_{J_n,J_{n-1}} \cdots \eta_{J_n,J_1}\eta_{J_n,K_{n-1}} \cdots \eta_{J_n,K_1})$$

therefore obtains the form given in Eq. (36) of the main text.

Appendix B. Generating functional and holomorphic representation

This derivation extends the works [30, 11] to the general case of a mixture of bosons and fermions. In the holomorphic representation the canonical operators are represented by

$$a^\dagger_p \to z_p$$

$$a_p \to \partial_{z_p} = \frac{\partial}{\partial z_p}$$

where z_p is an ordinary complex variable for bosonic index, and otherwise a complex Grassmann variable, and ∂_{z_p} is the left derivative. They satisfy the canonical graded commutation rules. In the following operators are denoted by capital letters, and their holomorphic or configuration-index representations by lower-case letters. The ket and bra states will be represented by the holomorphic functionals $f[z]$ and $\tilde{f}[\tilde{z}]$ where eventually $\tilde{z}_p = \partial_{z_p}$. If applied to continuous field theory, $z(x)$ is a complex- and possibly Grassmann-valued function, and $\delta/\delta z(x)$ the functional derivative. In the latter case, the information on the particle species and other internal degrees of freedom may be thought to be incorporated in the argument x and in the volume element dx, although additional indices would improve clarity.

The expectation value of an operator $O[a^\dagger, a]$ is, assuming normalization,

$$\langle O \rangle = \langle 0 | \tilde{f}[a] O[a^\dagger, a] f[a\dagger] | 0 \rangle = \tilde{f}[\partial_z] o[z, \partial_z] f[z]\big|_{z=0}. \qquad \text{(B1)}$$

The connection to the configuration notation of Sect. 3 can be specified more precisely as

$$F \Rightarrow f[z] = \sum_I C_I^\dagger[z] f_I = \sum_{\{m_p\}} \prod_{p\rightarrow} (z_p^{m_p}) f[m], \tag{B2}$$

where the configuration indices I are identified with the sets of exponents $\{m_p\}$, but normalization convention is slightly altered. The scalar product is then $\tilde{f}[\partial_z] f[z]|_{z=0} = \sum_{\{m_p\}} \tilde{f}[m] f[m] \prod_p (m_p!)$. The arrow notation above denotes a prescribed ordering of the factors. Similar representations are used also for the operators S, Σ, $\tilde{S}$ and $\tilde{\Sigma}$.

An exponential generating functional for normal ordered averages can be introduced as:

$$A[\tilde{u}, u] \equiv \langle e^{\langle \tilde{u} a^\dagger \rangle} e^{\langle u a \rangle} \rangle = \langle e^{\langle \tilde{u} z \rangle} e^{\langle u \partial_z \rangle} \rangle, \tag{B3}$$

where the bracket notation denotes the summation $\langle \tilde{u} z \rangle = \sum_p \tilde{u}_p z_p$, or the integration $\langle \tilde{u} z \rangle = \int dx \tilde{u}(x) z(x)$, if the formalism is applied to continuous field theory. The Grassmann parity of u_p and $\tilde{u}_p$ is determined by the index p. Thus the exponents are Grassmann-even. If an operator O is given in normal order, $O[a^\dagger, a] = :O[a^\dagger, a]:$, its average value can be calculated as follows:

$$\langle O[a^\dagger, a] \rangle = O[\partial_{\tilde{u}}, \partial_u] A[\tilde{u}, u]|_{\tilde{u}=u=0}. \tag{B4}$$

For example:

$$\left\langle \prod_{p\rightarrow} (a_p^{\dagger m_p}) \prod_{\leftarrow q} (a_q^{n_q}) \right\rangle = \tilde{f}[\partial_z] \prod_{p\rightarrow} (z_p^{m_p}) \prod_{\leftarrow q} (\partial_{z_q}^{n_q}) f[z] \Big|_{z=0}$$

$$= \prod_{p\rightarrow} (\partial_{\tilde{u}_p})^{m_p} \prod_{\leftarrow q} (\partial_{u_q})^{n_q} A[\tilde{u}, u] \Big|_{\tilde{u}=u=0}, \tag{B5}$$

where the oppositely directed arrows denote opposite orderings in the products.

The operators F, $\tilde{F}$, S etc. are Grassmann-even. Therefore, using the facts that:

$$\begin{aligned} \partial_{z_p} e^{\langle \tilde{u} z \rangle} &= e^{\langle \tilde{u} z \rangle} (\partial_{z_p} + \eta_p \tilde{u}_p) \\ e^{\langle u \partial_z \rangle} z_p &= (z_p + u_p) e^{\langle u \partial_z \rangle}, \end{aligned} \tag{B6}$$

the CIM expectation values are generated from:

$$A[\tilde{u}, u] = \tilde{f}[\partial_z + \eta \tilde{u}] f[z + u]|_{z=0}. \tag{B7}$$

This can be immediately translated into the CC methods:

$$A[\tilde{u}, u] = \tilde{s}[\partial_z + \eta \tilde{u}] e^{-s[z] + s[z+u]}|_{z=0}, \tag{B8}$$

where $\tilde{s}[\tilde{z}] = \exp \tilde{\sigma}[\tilde{z}]$.

Following the analysis of Refs. [30, 11] the coupled-cluster function $s[z]$ is represented by the analytic continuation of a functional Fourier transformation:

$$s[z] = \int \mathscr{D}\xi g[\xi] (e^{\langle z \xi \rangle} - 1), \tag{B9}$$

where $\mathscr{D}\xi = \prod_p d\xi_p$. The Grassmann parity of ξ_p is determined by the index p, and the integral over Grassmann variables is defined in the standard fashion. For

field theory $\mathscr{D}\xi(x)$ is the volume element in the function space. The product $\mathscr{D}\xi g[\xi]$ is Grassmann-even. In fact, both factors can be separately assumed even by considering only cases where the number of fermionic single-particle indices in $\mathscr{I}_1$ is even. The existence of the above Fourier transformation has been demonstrated for the case of anharmonic oscillators. Using Eqs. (B6) and (B9) the function $\sigma[z]$ can be expressed as

$$\begin{aligned}\sigma[z] &= \tilde{s}[\partial_z]s[z] - \tilde{s}[\partial_z]s[z]\big|_{z=0} \\ &= \int \mathscr{D}\xi\gamma[\xi](e^{\langle z\xi\rangle} - 1),\end{aligned} \tag{B10}$$

where

$$\gamma[\xi] = \tilde{s}[\xi]g[\xi]. \tag{B11}$$

For the anharmonic oscillator and comparable models the functions g and γ turn out to be generalized functions, which are singular at the origin ($\xi = 0$). In the case of field theories it is expected that they are generalized functionals.

The usual configuration representations s_I, σ_I for the operators S, Σ are obtained as *moments* of the distributions $g[\xi]$ and $\gamma[\xi]$, respectively, according to the generic rule

$$\sigma[m] = \int \mathscr{D}\xi\gamma[\xi] \prod_{\leftarrow p} \left[\frac{1}{m_p!}\xi_p^{m_p}\right]. \tag{B12}$$

The ECCM generating functional for the general case is obtained using Eqs. (B8–B11) with the result, written fully to emphasize the dependence of A on the state functionals $\tilde{\sigma}$ and γ,

$$\begin{aligned}A[\tilde{u}, u; \tilde{\sigma}, \gamma] = \sum_{n=0}^{\infty} \frac{1}{n!} \int \mathscr{D}\xi^1\gamma[\xi^1](e^{\langle u\xi^1\rangle} - 1) \cdots \int \mathscr{D}\xi^n\gamma[\xi^n](e^{\langle u\xi^n\rangle} - 1) \\ \cdot \exp\{\tilde{\sigma}[\eta\tilde{u} + \xi^1 + \cdots + \xi^n] - \tilde{\sigma}[\xi^1] - \cdots - \tilde{\sigma}[\xi^n]\}.\end{aligned} \tag{B13}$$

From this expansion only a finite number of terms are needed to calculate the averages of operators that are finite-order multinomials of the canonical operators. As an example, the model energy of Eq. (14) is in this representation

$$\bar{T} = \sum_p \int \mathscr{D}\xi\gamma[\xi]\xi_p t_p \frac{\delta}{\delta\xi_p}\tilde{\sigma}[\xi]. \tag{B14}$$

The full action functional is now (cf. Sect. 6)

$$\mathscr{A} = \int dt \left\{ i \int \mathscr{D}\xi\tilde{\sigma}[\xi]\dot{\gamma}[\xi] - \bar{H}[\tilde{\sigma}, \gamma] \right\}. \tag{B15}$$

Stationary conditions give in this representation the equations of motion

$$\begin{aligned}i\dot{\gamma}[\xi] &= \frac{\delta\bar{H}}{\delta\tilde{\sigma}[\xi]}, \\ i\dot{\tilde{\sigma}}[\xi] &= -\frac{\delta\bar{H}}{\delta\gamma[\xi]}.\end{aligned} \tag{B16}$$

The solutions corresponding to the ground state are obtained from these equations by setting the left-hand sides equal to zero.

Appendix C. Wick theorem

It is sufficient to prove the Wick theorem of Eqs. (54–55) for fermionic single-particle operators only. The bosonic operators completely factorize from the fermionic ones, and for that case the Wick theorem was proven in Ref. [22]. For any mixture of particles the rule will then be given in the present paper, assuming the model state to be the vacuum for all bosonic sectors.

Let $I=(i_1, i_2, i_3, \ldots), J=(j_1, j_2, j_3, \ldots)$, where all i_l or j_l are $\{0, 1\}$, and

$$\begin{aligned} C_I^\dagger &= a_1^{\dagger i_1} a_2^{\dagger i_2} a_3^{\dagger i_3} \cdots, \\ C_J &= \cdots a_3^{j_3} a_2^{j_2} a_1^{j_1}. \end{aligned} \tag{C1}$$

On arranging operators belonging to same orbitals into pairs it follows

$$C_J C_I^\dagger = K(a_1^{j_1} a_1^{\dagger i_1})(a_2^{j_2} a_2^{\dagger i_2}) \cdots,$$

where the sign factor is

$$K = \eta_J \eta_{I,J} (-1)^{(i_1+j_1)j_1 + (i_2+j_2)(j_1+j_2) + (i_3+j_3)(j_1+j_2+j_3) + \cdots}.$$

Using the elementary normal-ordering rule

$$a_1^{j_1} a_1^{\dagger i_1} = \sum_{k_1=0}^{\min(i_1, j_1)} \eta_{k_1} \eta_{i_1, j_1} a_1^{\dagger i_1 - k_1} a_1^{j_1 - k_1},$$

the pairs in the product $C_J C_I^\dagger$ can be normal-ordered. Shifting all the annihilation operators then to the right one obtains

$$C_J C_I^\dagger = K' \sum_{\{k_l\}} a_1^{\dagger i_1 - k_1} a_2^{\dagger i_2 - k_2} \cdots a_2^{j_2 - k_2} a_1^{j_1 - k_1}, \tag{C2}$$

where the sign factor is simplified into the form

$$\begin{aligned} K' = \eta_{i_i, j_1} \eta_{i_2, j_2} \cdots \eta_{k_1} \eta_{k_2} \cdots \eta_{I,K} \eta_{J,K} (-1)^{i_2 j_1 + i_3 (j_1 + j_2) + i_4 (j_1 + j_2 + j_3) + \cdots} \\ \cdot (-1)^{j_2 i_1 + j_3 (i_1 + i_2) + j_4 (i_1 + i_2 + i_3) + \cdots} (-1)^{k_1 (i_1 + j_1) + k_2 (i_1 + i_2 + j_1 + j_2) + \cdots}. \end{aligned} \tag{C3}$$

Operators with compound indices are calculated from the definition

$$\langle 0 | C_{J-K} \equiv \langle 0 | C_J C_K^\dagger = \langle 0 | \cdots a_2^{j_2} a_1^{j_1} a_1^{\dagger k_1} a_2^{\dagger k_2} \cdots,$$

which gives, after reordering,

$$C_{J-K} = \cdots a_2^{j_2 - k_2} a_1^{j_1 - k_1} (-1)^{k_2 (j_1 + k_1) + k_3 (j_1 + j_2 + k_1 + k_2) + \cdots}. \tag{C4}$$

In the same fashion one obtains

$$C_{I-K}^\dagger = a_1^{\dagger i_1 - k_1} a_2^{\dagger i_2 - k_2} \cdots (-1)^{k_2 (i_1 + k_1) + k_3 (i_1 + i_2 + k_1 + k_2) + \cdots}. \tag{C5}$$

Combining Eqs. (C4–C5) it is then found

$$C_{I-K}^\dagger C_{J-K} = a_1^{\dagger i_1 - k_1} a_2^{\dagger i_2 - k_2} \cdots a_2^{j_2 - k_2} a_1^{j_1 - k_1} (-1)^{k_2 (i_1 + j_1) + k_3 (i_1 + i_2 + j_1 + j_2) + \cdots}. \tag{C6}$$

On comparing Eqs. (C2–C3) with (C6) one finds

$$C_J C_I^\dagger = \sum_{\{k_l\}} C_{I-K}^\dagger C_{J-K} Z_K(I, J), \tag{C7}$$

where the sign factor is

$$Z_K(I, J) = \eta_{i_1, j_1} \eta_{i_2, j_2} \cdots \eta_{k_1} \eta_{k_2} \cdots \eta_{I,K} \eta_{J,K} (-1)^{\sum_{l \neq m} i_l j_m} (-1)^{\sum_l k_l (i_l + j_l)}.$$

But $(-1)^{\sum_{l\neq m} i_l j_m} = (-1)^{N_I N_J + \sum_l i_l j_l} = \eta_{I,J} \prod_l \eta_{i_l,j_l}$. Therefore

$$Z_K(I,J) = \eta_{I,J}\eta_{I,K}\eta_{J,K} \prod_l (\eta_{k_l}\eta_{k_l,i_l}\eta_{k_l,j_l}).$$

A closer inspection shows that for all possible configurations $\eta_{k_l}\eta_{k_l,i_l}\eta_{k_l,j_l} = \eta_{k_l}$ Therefore the product of all these factors is η_K, which finally proves Eqs. (54–55) of the main text.

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