Non-Hermitian coupled cluster method for non-stationary systems and its interaction-picture reinterpretation

Document Version
Final published version

[Link to publication record in Manchester Research Explorer](#)

Citation for published version (APA):
Bishop, R. F., & Znojil, M. (2020). Non-Hermitian coupled cluster method for non-stationary systems and its interaction-picture reinterpretation. *European Physical Journal Plus*, *135*, [374 (35pp)]. https://doi.org/10.1140/epjp/s13360-020-00374-z

Published in:
European Physical Journal Plus

Citing this paper
Please note that where the full-text provided on Manchester Research Explorer is the Author Accepted Manuscript or Proof version this may differ from the final Published version. If citing, it is advised that you check and use the publisher's definitive version.

THE EUROPEAN
PHYSICAL JOURNAL PLUS

Non-Hermitian coupled cluster method for non-stationary systems and its interaction-picture reinterpretation

R. F. Bishop[1,2,3,a] , **M. Znojil**[4,5,6,b]

[1] Department of Physics and Astronomy, Schuster Building, The University of Manchester, Manchester M13 9PL, UK
[2] Quantum Systems Engineering Research Group, Department of Physics, Loughborough University, Leicestershire LE11 3TU, UK
[3] School of Physics and Astronomy, University of Minnesota, 116 Church Street SE, Minneapolis, MN 55455, USA
[4] The Czech Academy of Sciences, Nuclear Physics Institute, Hlavní 130, 250 68 Řež, Czech Republic
[5] Department of Physics, Faculty of Science, University of Hradec Králové, Rokitanského 62, 500 03 Hradec Králové, Czech Republic
[6] Institute of System Science, Durban University of Technology, P. O. Box 1334, Durban 4000, South Africa

Abstract The interaction picture in a non-Hermitian realization is discussed in detail and considered for its practical use in many-body quantum physics. The resulting non-Hermitian interaction-picture (NHIP) description of dynamics, in which both the wave functions and operators belonging to physical observables cease to remain constant in time, is a non-Hermitian generalization of the traditional Dirac picture of standard quantum mechanics, which itself is widely used in quantum field theory calculations. Particular attention is paid here to the variational (or, better, bivariational) and dynamical (i.e., non-stationary) aspects that are characteristic of the coupled cluster method (CCM) techniques that nowadays form one of the most versatile and most accurate of all available formulations of quantum many-body theory. In so doing we expose and exploit multiple parallels between the NHIP and the CCM in its time-dependent versions.

1 Introduction

In a wide variety of branches of applied quantum mechanics, one often needs to know, with a reasonable numerical precision, the value and evolution of the time-dependent wave function $\psi(t)$. Not surprisingly, the construction of this function is relatively straightforward only for a few exceptional, not too complicated (and hence also, generically, not very realistic) self-adjoint Hamiltonians $\mathfrak{h}$ in the Schrödinger equation (in units where $\hbar = 1$ throughout),

$$i\partial_t \psi(t) = \mathfrak{h}\,\psi(t)\,. \tag{1}$$

---

[a] e-mail: raymond.bishop@manchester.ac.uk (corresponding author)

[b] e-mail: znojil@ujf.cas.cz

Springer

The task usually requires the use of one of the available sophisticated (e.g., typically, perturbative or variational) numerical methods. In the present paper we recall two of the apparently very different strategies of the variational class, with the express intention of showing that behind the apparent formal differences one can also find multiple parallels that can lead to new ideas and novel constructive approaches.

The present study has its roots in our earlier investigation [1] in which we succeeded in comparing some alternative methods of solving Eq. (1) in the stationary regime, in each of which the construction remains reducible to the diagonalization of the Hamiltonian $\mathfrak{h}$. In particular we revealed a close structural parallelism between the powerful and versatile coupled cluster method (CCM) approach to the diagonalization of operator $\mathfrak{h}$ (and see, e.g., Refs. [2–6] for details of the formalism) and the successful interacting boson model (IBM) [7–9]. The CCM is, by now, well known and very widely used in such fields as atomic and molecular physics, nuclear physics, quantum chemistry (in which it forms the "gold standard" for accuracy), and many branches of condensed matter physics, while the IBM offers an efficient tool for the calculation of the low-lying spectra of energies E of the heaviest stable atomic nuclei [7–9].

In the present paper our aim is to demonstrate that the above-mentioned parallelism finds its further natural extension to the domain of dynamics in which the quantum systems in question are non-stationary. We shall first recall the known CCM $\leftrightarrow$ IBM parallels [1], and then show how to generalize them. We do so along lines that are guided by the expectation of a mutual enrichment. Explicitly, for the numerical constructions of energies E and wave functions $\psi(t)$, we pay specific attention here to two specific alternative strategies, viz. the various versions of the CCM approach (see, e.g., Ref. [10] for a compact introductory review) and to standard (or "textbook") quantum theory in its so-called three-Hilbert-space formulation [11,12]. For a comprehensive introduction to some of the most successful phenomenological applications of the three-Hilbert-space formalism the reader is also referred to Refs. [13,14].

We anticipate that the future impact of our considerations might range from a purely mathematical guarantee of the computational feasibility of model-building, up to a deeply physical reinterpretation of relationships between alternative formulations of many-body quantum mechanics. We will emphasize certain emergent features of connections between different means of description and between the simplifying assumptions and dynamics-simulating techniques.

2 The fundamentals of the CCM approach

None of the existing CCM-based calculations leaves the traditional theoretical framework of quantum mechanics. The correspondence between the IBM and CCM formulations of quantum mechanics may be one-to-one. Indeed, both formulations employ the factorized Ansatz

$$\psi = \Omega \, \psi_0 \,, \tag{2}$$

in which the auxiliary (and, generally, non-unitary) operator Ω is intended to serve as the source of the quantum correlations which are unaccounted for in the original approximation ψ_0. One of the most natural mathematical requirements imposed upon the operator Ω is that it should be *invertible*. Thus, the element ψ of an initial physical Hilbert space $\mathcal{H}^{\text{(initial)}}$ is treated as an image of a, presumably, *perceivably simpler* reference state ψ_0, which may itself belong, in principle, to another, more user-friendly, auxiliary Hilbert space $\mathcal{H}^{\text{(user–friendly)}}$. The original Hamiltonian $\mathfrak{h}$ of Eq. (1) belonging to $\mathcal{H}^{\text{(initial)}}$ is similarly replaced by its

isospectral (and, in general, non-Hermitian) avatar,

$$H = \Omega^{-1} \mathfrak{h} \Omega \, , \tag{3}$$

that belongs to the auxiliary Hilbert space $\mathcal{H}^{\text{(user–friendly)}}$.

In the CCM setting, the auxiliary operator Ω in the Ansatz of Eq. (2) takes the very specific exponentiated form,

$$\Omega = \exp S \, . \tag{4}$$

This characteristic feature of the method henceforth ensures that the Goldstone linked cluster theorem [15] is automatically satisfied for the system under study at any level of approximation for the operator S, as we explain in more detail below. In turn, this guarantees the very important property for all many-body systems that at all such levels the system is both size-extensive and size-consistent [10], where size-extensivity is the property that the leading term in the energy of an N-particle self-bound system scales linearly with N as $N \to \infty$, and where size-consistency implies that a many-body wave function dissociates correctly into non-interacting fragments under infinite separation of the fragments.

The original version of the CCM, as invented independently by Coester and Kümmel [16,17] and Čížek [18,19], is nowadays referred to as the normal CCM (NCCM), in order to distinguish it from the later extended (ECCM) version introduced by Arponen [2]. For present purposes most of what we discuss here is equally relevant to both versions, although we mostly have the NCCM in mind for specific applications.

2.1 The normal coupled cluster method (NCCM)

The exact ket and bra wave functions for an arbitrary quantum many-body system are defined in $\mathcal{H}^{\text{(initial)}}$ to be $|\psi(t)\rangle$ and

$$\langle \tilde{\psi}(t)| \equiv \frac{\langle \psi(t)|}{\langle \psi(t)|\psi(t)\rangle} \, , \tag{5}$$

respectively, at an arbitrary time t. We assume that the Hilbert space $\mathcal{H}^{\text{(initial)}}$ for the system may be described in terms of a normalized, stationary reference (or model) state $|\psi_0\rangle$ (i.e., with $\langle \psi_0|\psi_0\rangle = 1$), just as in Eq. (2). Within the CCM we further assume that the reference state acts as a cyclic vector for a corresponding set of *mutually commuting* multi-configurational creation operators $\{C_I^+\}$,

$$[C_I^+, C_J^+] = 0 \, ; \quad \forall I, J \, , \tag{6}$$

such that $|\psi_0\rangle$ acts as a *generalized vacuum state* with respect to them,

$$C_I^-|\psi_0\rangle = 0 = \langle \psi_0|C_I^+ \, ; \quad \forall I \neq 0 \, , \tag{7}$$

in a notation where we define $C_I^- \equiv (C_I^+)^\dagger$ and $C_0^+ \equiv \mathbb{1}$, the unit vector. The reference state $|\psi_0\rangle$ must also be chosen to be non-orthogonal to the actual wave function $|\psi(t)\rangle$ of the system,

$$\langle \psi_0|\psi(t)\rangle \neq 0 \, ; \quad \forall t \, . \tag{8}$$

The index I is a set index and, in general, the multi-configurational creation operator C_I^+ comprises a product of single-particle operators, as we illustrate in Sect. 2.3 for a specific example. The set $\{I\}$ is complete in the usual sense that the set of states $\{C_I^+|\psi_0\rangle\}$ provides

a complete basis for the ket Hilbert space. It is also convenient to choose the basis to be orthonormalized, such that

$$\langle \psi_0 | C_I^- C_J^+ | \psi_0 \rangle = \delta_{I,J} \,, \tag{9}$$

where $\delta_{I,J}$ is an appropriately defined Kronecker symbol. In this case we have that the identity operator in the Hilbert space may be resolved as

$$\sum_I C_I^+ | \psi_0 \rangle \langle \psi_0 | C_I^- = \mathbb{1} = | \psi_0 \rangle \langle \psi_0 | + \sum_{I \neq 0} C_I^+ | \psi_0 \rangle \langle \psi_0 | C_I^- \,. \tag{10}$$

The ket and bra states of the many-body system are now formally parametrized *independently* in the NCCM as follows,

$$|\psi(t)\rangle \equiv e^{k(t)} e^{S(t)} |\psi_0\rangle \,, \quad \langle \tilde{\psi}(t)| \equiv e^{-k(t)} \langle \psi_0 | \tilde{S}(t) e^{-S(t)} \,, \tag{11}$$

in terms of the *c*-number function $k(t)$, and the NCCM time-dependent correlation operators $S(t)$ and $\tilde{S}(t)$, which are themselves now decomposed as follows,

$$S(t) = \sum_{I \neq 0} s_I(t) C_I^+ \,, \quad \tilde{S}(t) = \mathbb{1} + \sum_{I \neq 0} \tilde{s}_I(t) C_I^- \,. \tag{12}$$

The scale factor $k(t)$ is needed for the temporally evolving intermediate normalization (i.e., $\langle \psi_0 | \psi(t) \rangle = e^{k(t)}$) but is irrelevant henceforth since it cancels from any expectation value [and the normalization condition $\langle \tilde{\psi}(t) | \psi(t) \rangle = 1$ from Eq. (5) is now preserved for all times t] by the specific parametrizations of Eqs. (11) and (12). Since $S(t)$ and $\tilde{S}(t)$ are henceforth treated as independent operators, the Hermiticity relation between corresponding ket and bra states may be violated when subsequent approximations are made, typically by truncating the complete set of configurations $\{I\}$ in the sums of Eq. (12). This shortcoming is far outweighed by the fact that the CCM parametrizations of Eqs. (11) and (12) always *exactly* satisfy the very important Hellmann–Feynman theorem [20,21] at all such levels of approximation [10]. It is precisely this feature that guarantees the robustness and accuracy of numerical results obtained within the CCM framework.

The expectation value $\overline{Q}(t)$ of an arbitrary physical observable described by the Hermitian operator $\mathfrak{q}(t)$ in $\mathcal{H}^{(\text{initial})}$, which may itself have an intrinsic time dependence, may thus be expressed within the NCCM wholly in terms of the set of *c*-number correlation coefficients $\{s_I(t), \tilde{s}_I(t)\}$ as follows,

$$\langle \mathfrak{q}(t) \rangle = \overline{Q}(t) = \overline{Q}[s_I, \tilde{s}_I; t] \equiv \langle \psi_0 | \tilde{S}(t) e^{-S(t)} \mathfrak{q}(t) e^{S(t)} | \psi_0 \rangle \,. \tag{13}$$

Such an expectation functional is evaluated by employing the nested commutation expansion for the similarity transform $Q(t)$ [c.f., Eq. (3)] which is just the NCCM avatar in $\mathcal{H}^{(\text{user–friendly})}$ of the operator $\mathfrak{q}(t)$ in $\mathcal{H}^{(\text{initial})}$,

$$Q(t) \equiv e^{-S(t)} \mathfrak{q}(t) e^{S(t)} \tag{14a}$$

$$= \sum_{n=0}^{\infty} \frac{1}{n!} [\mathfrak{q}(t), S(t)]_n \,. \tag{14b}$$

Here, the *n*-fold nested commutators $[\mathfrak{q}, S]_n$ are defined iteratively,

$$[\mathfrak{q}, S]_n = [[\mathfrak{q}, S]_{n-1}, S] \,, \quad [\mathfrak{q}, S]_0 \equiv \mathfrak{q} \,. \tag{15}$$

The similarity-transformed Hamiltonian, $H(t) \equiv e^{-S(t)} \mathfrak{h} e^{S(t)}$, lies at the heart of the NCCM. Its parametrizations of Eqs. (11) and (12) are specifically chosen so that the otherwise infinite

sum in Eq. (14b) will actually terminate exactly at a low finite order for any operator q all of whose terms involve only a product of a finite number of single-particle operators, such as is almost always the case for the operators of interest. The reason for this termination lies simply in the twin facts that all components of the operator $S(t)$ in the expansion of Eq. (12) commute with one another from Eq. (6), and the basic single-particle operators form a Lie algebra, together with the model state $|\psi_0\rangle$ being a vacuum state for the operator set $\{C_I^+\}$, as in Eq. (7) (and see, e.g., Refs. [6,10] for further details).

The above same key feature of the NCCM is also responsible for all terms in the expansion of $\overline{Q}(t)$ from Eq. (13) for any physical operator q being *linked*. Thus, we may write the NCCM expectation value functional $\overline{Q}(t)$ in the schematic form,

$$\overline{Q}[s_I, \tilde{s}_I; t] = \sum_{n=0}^{\infty} \frac{1}{n!} \sum_J \sum_{K_1 \neq 0} \cdots \sum_{K_n \neq 0} \langle J | \mathfrak{q}(t) | K_1, \cdots, K_n \rangle_{\mathrm{NCCM}} \tilde{s}_J s_{K_n} \cdots s_{K_1}, \quad (16)$$

where, by comparison with Eqs. (14b) and (15), the NCCM matrix elements may be written as

$$\langle J | \mathfrak{q}(t) | K_1, \ldots, K_n \rangle_{\mathrm{NCCM}} \equiv \langle \psi_0 | C_J^- \, \mathfrak{q}(t) \, C_{K_1}^+ \cdots C_{K_n}^+ | \psi_0 \rangle_{\mathcal{L}} . \quad (17)$$

The suffix $\mathcal{L}$ in Eq. (17) indicates the NCCM *linked* structure implied by the nested commutator sum, viz. that from each group of particles characterized by each of the configuration-space indices K_j, the amplitude s_{K_j} associated with the cluster creation operator $C_{K_j}^+$, must have at least one particle line connected to the operator q. After expanding Eq. (13) in powers of S by the use of Eq. (14b), only such terms are retained where at least one link (or contraction, due to a non-vanishing commutator term) exists between each S operator and the operator q. The sum over n in Eq. (16) will extend again to a finite limit depending on the operator q.

It is precisely this linkedness feature (specifically for the energy expectation value functional $\overline{H}(t)$), as expressed in Eqs. (16) and (17), that implies immediately that the NCCM automatically satisfies exactly the Goldstone linked-cluster theorem [15] at any level of truncation in the expansions of Eq. (12) for the correlation operators. In turn this also immediately guarantees the size-extensivity of the method at all such levels of approximation. Thus, in the solution of the explicit evolution equations that we will now derive for the basic NCCM amplitudes $\{s_I(t), \tilde{s}_I(t)\}$, the only approximation that is ever made in any CCM calculation is to decide which configurations $\{I\}$ are to be retained in the expansions of Eq. (12).

The NCCM coefficients $\{s_I(t), \tilde{s}_I(t)\}$ are obtained by introducing the action functional $\mathcal{A}$,

$$\mathcal{A} \equiv \int_{t_0}^{t_1} \mathrm{d}t \, \langle \tilde{\psi}(t) | \, (\mathrm{i}\partial/\partial t - \mathfrak{h}) \, | \psi(t) \rangle . \quad (18)$$

The (bivariational) stationarity principle,

$$\frac{\partial \mathcal{A}}{\partial \langle \tilde{\psi}(t) |} = 0 = \frac{\partial \mathcal{A}}{\partial | \psi(t) \rangle} , \quad (19)$$

with respect to all independent variations in the bra and ket states, subject to the conditions $\delta \langle \tilde{\psi}(t_i) | = 0 = \delta | \psi(t_i) \rangle$ where $i = 0, 1$, is seen to be equivalent to the time-dependent Schrödinger equations,

$$\mathrm{i}\partial_t | \psi(t) \rangle = \mathfrak{h} \, \psi(t) , \quad -\mathrm{i}\partial_t \langle \tilde{\psi}(t) | = \langle \tilde{\psi}(t) | \mathfrak{h} , \quad (20)$$

analogous to Eq. (1). Insertion of the NCCM parametrizations of Eqs. (11) and (12) into Eq. (18) yields the result,

$$
\mathcal{A} = \int_{t_0}^{t_1} dt \left\{ i \sum_{I \neq 0} \left(\tilde{s}_I \frac{ds_I}{dt} \right) - \overline{H}[s_I, \tilde{s}_I] \right\} = \int_{t_0}^{t_1} dt \left\{ -i \sum_{I \neq 0} \left(\frac{d\tilde{s}_I}{dt} s_I \right) - \overline{H}[s_I, \tilde{s}_I] \right\}. \tag{21}
$$

The independent (bivariational) stationarity conditions, $\partial \mathcal{A} / \partial \tilde{s}_I = 0 = \partial \mathcal{A} / \partial s_I$, then yield the evolution equations for the NCCM cluster correlation coefficients,

$$
i \frac{ds_I}{dt} = \frac{\partial \overline{H}}{\partial \tilde{s}_I}, \quad -i \frac{d\tilde{s}_I}{dt} = \frac{\partial \overline{H}}{\partial s_I}; \quad \forall I \neq 0, \tag{22}
$$

in terms of the energy expectation functional $\overline{H}$, given as in Eq. (13) with the replacement $\mathfrak{q}(t) \to \mathfrak{h}$. We recognize these equations as (being closely related to) the *classical* Hamilton's equations of motion for the NCCM cluster correlation coefficients. Thus, the coefficients s_I and $\tilde{s}_I$ form *canonically conjugate pairs* in the usual sense of classical mechanics.

We can now also easily derive the equation of motion for the expectation value $\overline{Q}(t) \equiv \overline{Q}[s_I, \tilde{s}_I; t]$ of an arbitrary operator $\mathfrak{q}(t)$ in $\mathcal{H}^{(\text{initial})}$ given by Eq. (13). Using Eq. (22), we rewrite the usual chain-rule relation,

$$
\frac{d\overline{Q}}{dt} = \frac{\partial \overline{Q}}{\partial t} + \sum_{I \neq 0} \left(\frac{\partial \overline{Q}}{\partial s_I} \frac{ds_I}{dt} + \frac{\partial \overline{Q}}{\partial \tilde{s}_I} \frac{d\tilde{s}_I}{dt} \right), \tag{23}
$$

in the suggestive form,

$$
\frac{d\overline{Q}}{dt} = \frac{\partial \overline{Q}}{\partial t} + \{\overline{Q}, \overline{H}\}, \tag{24}
$$

in terms of a generalized *classical Poisson bracket*, defined between the expectation values $\overline{A}$ and $\overline{B}$ of two arbitrary operators in $\mathcal{H}^{(\text{user-friendly})}$ as follows,

$$
\{\overline{A}, \overline{B}\} \equiv \frac{1}{i} \sum_{I \neq 0} \left(\frac{\partial \overline{A}}{\partial s_I} \frac{\partial \overline{B}}{\partial \tilde{s}_I} - \frac{\partial \overline{A}}{\partial \tilde{s}_I} \frac{\partial \overline{B}}{\partial s_I} \right). \tag{25}
$$

Equation (24) is just the well-known classical equation of motion in the canonical formalism. It is clearly the classical, *exactly mapped*, counterpart of the usual quantum-mechanical Heisenberg equation of motion for the operator $\mathfrak{q}(t)$ in the original Hilbert space $\mathcal{H}^{(\text{initial})}$,

$$
\frac{d\mathfrak{q}}{dt} = \frac{\partial \mathfrak{q}}{\partial t} + \frac{1}{i} [\mathfrak{q}, \mathfrak{h}], \tag{26}
$$

with the lower-case operator $\mathfrak{q}(t)$ and its upper-case NCCM similarity-transformed avatar operator $Q(t)$ related by Eq. (14a)

The above results can be made even more suggestive by choosing new basic variables to be the generalized *c*-number fields ϕ_I and their canonically conjugate *c*-number generalized momentum densities π_I, which are defined as follows,

$$
\phi_I \equiv 2^{-1/2}(s_I + \tilde{s}_I); \quad \pi_I \equiv -i\, 2^{-1/2}(s_I - \tilde{s}_I). \tag{27a}
$$

The inverse transformations are thus simply given by

$$
s_I \equiv 2^{-1/2}(\phi_I + i\pi_I); \quad \tilde{s}_I \equiv 2^{-1/2}(\phi_I - i\pi_I). \tag{27b}
$$

It is now easy to show that Eq. (25) in the new variables takes the following form,

$$\{\overline{A}, \overline{B}\} = \sum_{I \neq 0} \left(\frac{\partial \overline{A}}{\partial \phi_I} \frac{\partial \overline{B}}{\partial \pi_I} - \frac{\partial \overline{A}}{\partial \pi_I} \frac{\partial \overline{B}}{\partial \phi_I} \right) . \tag{28}$$

The equations of motion (22) lead to their equivalent counterparts for the new variables,

$$\frac{d\phi_I}{dt} = \frac{\partial \overline{H}}{\partial \pi_I} = \{\phi_I, \overline{H}\} ; \quad \forall I \neq 0 , \tag{29a}$$

$$\frac{d\pi_I}{dt} = -\frac{\partial \overline{H}}{\partial \phi_I} = \{\pi_I, \overline{H}\} ; \quad \forall I \neq 0 . \tag{29b}$$

The (completely classical) phase space $\{\phi_I, \pi_I\}$ has the canonical symplectic structure,

$$\begin{aligned} \{\phi_I, \pi_J\} &= \delta_{I,J} ; \quad \forall I \neq 0 , J \neq 0 , \\ \{\phi_I, \phi_J\} &= 0 = \{\pi_I, \pi_J\} . \end{aligned} \tag{30}$$

In order to complete this description of an exact *classicization* of an arbitrary quantum many-body theory, we note that the expectation value of the commutator between an *arbitrary* pair of operators $\mathfrak{a}$ and $\mathfrak{b}$ in the original Hilbert space $\mathcal{H}^{(\mathrm{initial})}$ is also *exactly* mapped into its corresponding Poisson bracket of Eq. (25) or Eq. (28). We may use Eq. (13) to write the expectation value of the product $\mathfrak{ab}$ of the two operators as

$$\langle \mathfrak{ab} \rangle = \langle \psi_0 | \tilde{S}(t) \mathrm{e}^{-S(t)} \mathfrak{ab} \mathrm{e}^{S(t)} | \psi_0 \rangle = \langle \psi_0 | \tilde{S}(t) \mathrm{e}^{-S(t)} \mathfrak{a} \mathrm{e}^{S(t)} \mathrm{e}^{-S(t)} \mathfrak{b} \mathrm{e}^{S(t)} | \psi_0 \rangle , \tag{31}$$

and hence, using Eq. (14a), as

$$\langle \mathfrak{ab} \rangle = \langle \psi_0 | \tilde{S}(t) A(t) B(t) | \psi_0 \rangle = \overline{AB} . \tag{32}$$

By inserting a resolution of the identity of the form of Eq. (10) between the operators $A(t)$ and $B(t)$ in the middle expression in the above equation, we find

$$\begin{aligned} \overline{AB} &= \sum_I \langle \psi_0 | \tilde{S}(t) A(t) C_I^+ | \psi_0 \rangle \langle \psi_0 | C_I^- B(t) | \psi \rangle \\ &= \sum_I \langle \psi_0 | \tilde{S}(t) [A(t), C_I^+] | \psi \rangle \langle \psi_0 | C_I^- B(t) | \psi_0 \rangle \\ &\quad + \sum_I \langle \psi_0 | \tilde{S}(t) C_I^+ A(t) | \psi_0 \rangle \langle \psi_0 | C_I^- B(t) | \psi_0 \rangle . \end{aligned} \tag{33}$$

The term with $I = 0$ in the sum in the first term of the above equation is identically zero, since $C_0^+ \equiv \mathbb{1}$. Next, if we use the explicit form for the expectation value of an arbitrary operator given by Eq. (13), together with the NCCM forms for the operators $S(t)$ and $\tilde{S}(t)$ given by Eq. (12), we finally derive the following relations for the remaining terms,

$$\frac{\partial \overline{Q}}{\partial \tilde{s}_I} = \langle \psi_0 | C_I^- Q(t) | \psi_0 \rangle ; \quad \forall I \neq 0 , \tag{34a}$$

$$\frac{\partial \overline{Q}}{\partial s_I} = \langle \psi_0 | \tilde{S}(t) [Q(t), C_I^+] | \psi_0 \rangle ; \quad \forall I \neq 0 . \tag{34b}$$

Substitution of Eqs. (34a) and (34b) into the second line of Eq. (33) then yields the following result,

$$
\langle \mathfrak{a}\mathfrak{b} \rangle = \overline{AB} = \sum_{I \neq 0} \frac{\partial \overline{A}}{\partial s_I} \frac{\partial \overline{B}}{\partial \tilde{s}_I}
$$
$$
+ \sum_I \sum_J \langle \psi_0 | \tilde{S}(t) C_I^+ C_J^+ | \psi_0 \rangle \langle \psi_0 | C_J^- A(t) | \psi_0 \rangle \langle \psi_0 | C_I^- B(t) | \psi_0 \rangle, \qquad (35)
$$

where in the third line of Eq. (33) we have inserted a resolution of the identity operator of the form of Eq. (10) between the operators C_I^+ and $A(t)$. The last term in Eq. (35) is symmetric under the interchange $A \rightleftarrows B$, as $[C_I^+, C_J^+] = 0$ from Eq. (6), and hence we arrive at the desired relation,

$$
\langle [\mathfrak{a}, \mathfrak{b}] \rangle = \overline{[A, B]} = \overline{AB} - \overline{BA} = \sum_{I \neq 0} \left(\frac{\partial \overline{A}}{\partial s_I} \frac{\partial \overline{B}}{\partial \tilde{s}_I} - \frac{\partial \overline{A}}{\partial \tilde{s}_I} \frac{\partial \overline{B}}{\partial s_I} \right) = i\{\overline{A}, \overline{B}\}. \qquad (36)
$$

It is very important to note that the consistency of the classical and quantum formulations induced by the NCCM can thus be understood as a manifestation of the correspondence principle (or Ehrenfest theorem) in a suitably generalized form.

In partial summary, we have thus been led to a key result of the NCCM formalism, namely that our (rather arbitrarily specified) quantum many-body problem in a Hilbert space has been exactly mapped onto the classical Hamiltonian mechanics for the complex c-number amplitudes $\{s_I, \tilde{s}_I\}$, or equivalently the canonical fields $\{\phi_I\}$ and their conjugate momentum densities $\{\pi_I\}$, in a classical NCCM phase space. These fields are themselves defined as many-body amplitudes in the configuration space labeled by the indices $\{I\}$ that describe the particular subsets (or clusters) of particles under consideration. In the modern terminology of classical mechanics this phase space is a symplectic differentiable manifold [22]. The differentiability is just a consequence of the fact that the c-number parameters $\{s_I, \tilde{s}_I\}$ or, equivalently, $\{\phi_I, \pi_I\}$, are continuous complex numbers, with respect to which one is allowed to take (possibly functional) derivatives. The symplectic nature of the phase space is a direct consequence of the existence of the generalized Poisson bracket, which is just a skew-symmetric bilinear form that can be used to define a Hamiltonian vector field in the tangent space of the manifold [22]. The set of trajectories defined by the equations of motion will fill the whole of the dynamically allowed region of the phase space.

The exact classicization mapping opens up the possibility of being able to exploit or to extend all of the techniques developed in classical mechanics for use in the quantum many-body problem. For example, one can make easy contact with *conservation laws* and the associated sum rules by using the Noether currents. It is also intuitively apparent from the existence of this mapping onto classical mechanics that the c-number NCCM amplitudes $\{\phi_I, \pi_I\}$ or $\{s_I, \tilde{s}_I\}$, which completely characterize and decompose our many-body problem, may be viewed as a set of *generalized mean fields* which describe each subsystem of particles in the interacting many-body system as labeled by the configuration-space indices $\{I\}$.

Let us now return briefly to the non-Hermitian nature of the NCCM approach. The requirement that the physical bra and ket states in the original Hilbert space $\mathcal{H}^{(\text{initial})}$ should be Hermitian conjugates of one another, implies from Eqs. (5) and (11) that

$$
\langle \psi_0 | \tilde{S} = \frac{\langle \psi_0 | e^{S^\dagger} e^S}{\langle \psi_0 | e^{S^\dagger} e^S | \psi_0 \rangle}, \qquad (37)
$$

and hence to constraints between the set of amplitudes $\{s_I, \tilde{s}_I\}$. Thus, the observable physical space is just a submanifold in the full NCCM symplectic phase space. It is, however, an invariant submanifold in the sense that it comprises entire trajectories, such that either none or all of the points of a trajectory belong to the physical submanifold, under the sole assumption that the original Hamiltonian $\mathfrak{h}$ in $\mathcal{H}^{(\text{initial})}$ is Hermitian. Temporal evolution thus leaves this submanifold invariant. Even within this submanifold the respective pairs of amplitudes s_I and $\tilde{s}_I$ are not in general complex conjugates of one another since the underlying NCCM similarity transformation is not unitary. These pairs of amplitudes are in no simple relationship to one another. Correspondingly, neither the generalized fields ϕ_I nor their canonically conjugate generalized momentum densities π_I, as defined in Eq. (27a) will in general be real. It is only by performing a suitable complex canonical transformation (i.e., a symplectomorphism) that one can regain a description in terms of manifestly real coordinates $\{\phi_I', \pi_I'\}$ instead of complex ones.

There are actually (at least) two different approaches to achieving the above aim. The first, and perhaps most direct, has been performed by Arponen [23], who first introduces the set of complex conjugate NCCM amplitudes $\{s_I^*, \tilde{s}_I^*\}$, whereby the NCCM phase space is enlarged into a genuine complex manifold, but self-evidently now of too large a dimensionality. Thus, finally, the extra degrees of freedom are explicitly eliminated by using the Dirac bracket method and deriving the induced symplectic structure, in order to construct the physical manifold (otherwise known as the constraint surface or physical shell), in which the remaining independent amplitudes are a minimal set of complex conjugate pairs or, equivalently, a manifestly real set $\{\phi_I', \pi_I'\}$. He shows that the NCCM physical shell is actually a Kähler manifold, and the constraint functions themselves are of second class [24], as is precisely the case in a gauge theory where the constraint corresponds precisely to a complete gauge fixing, even though in the NCCM case the constraints do not seem to correspond to any internal (hidden) gauge symmetries of the problem. The resulting reduced phase space of the physical shell is shown to be itself a complex manifold with a symplectic structure, just like the original extended phase space. The symplectic structure is given by an induced symplectic two-form, whose general form is derived without making any approximations or restricting assumptions. It has also been shown in Ref. [23] that the NCCM star product is well defined in the reduced phase space, or the constraint surface, where the star product is defined to give the expectation of a product of operators in terms of the expectations of individual operators, and where it is also shown that it is implemented by a certain tensor field of type $(2, 0)$.

The second approach to "re-Hermitizing" the NCCM formulation by a canonical transformation (i.e., a symplectomorphism) of the set of amplitudes $\{s_I, \tilde{s}_I\}$ (or, equivalently, $\{\phi_I, \pi_I\}$) has been performed more indirectly by diagonalizing the effective Hamiltonian that governs small oscillations around the equilibrium ground state [4]. It has been explicitly shown in Ref. [4] that this diagonalization procedure is equivalent to performing a canonical coordinate transformation into normal coordinates in the symplectic phase space. The normal frequencies are also then precisely the excitation energies. In terms of the new normal coordinates the Hamiltonian functional $\overline{H}$ thus recovers a manifestly Hermitian form that was lost in the original NCCM form of the functional $\overline{H}[s_I, \tilde{s}_I]$ due to the nonunitary nature of the similarity transformation that lies at the heart of the NCCM.

2.2 The extended coupled cluster method (ECCM)

Let us now briefly conclude our discussion of the CCM fundamentals by considering the extension of the above ideas to the ECCM. As we have seen, any NCCM expectation value functional $\overline{Q}(t) = \overline{Q}[s_I, \tilde{s}_I; t]$ comprises only linked (or connected) terms. The exponen-

tiated form of the NCCM ket-state correlation operator in Eq. (11) also guarantees that all of the coefficients $\{s_I; \forall I \neq 0\}$ are themselves fully linked. However, the corresponding canonically conjugate NCCM bra-state coefficients $\{\tilde{s}_I; \forall I \neq 0\}$ *do* contain unlinked terms. If and when needed, this can be remedied by introducing the following ECCM exponentiated form for the NCCM bra-state correlation operator, $\tilde{S}(t)$,

$$\tilde{S}(t) \equiv e^{\tilde{\Sigma}(t)}; \quad \tilde{\Sigma}(t) = \sum_{I \neq 0} \tilde{\sigma}_I(t) C_I^- . \tag{38}$$

It is clear from Eqs. (6), (12) and (13) that the NCCM cluster coefficients $\tilde{s}_I$ may be expressed as $\tilde{s}_I = \langle C_I^+ \rangle$, which in general are *not* linked quantities. The linked pieces of these expectation values that remain after the disconnected terms have been discarded are precisely the new ECCM cluster coefficients, $\tilde{\sigma}_I = \langle C_I^+ \rangle_{\text{linked}}$.

From Eqs. (7) and (38) we deduce that $\tilde{\Sigma}(t)|\psi_0\rangle = 0$ so that we may write the ECCM parametrizations of the ket and bra many-body wave functions as follows,

$$|\psi(t)\rangle \equiv e^{k(t)} e^{S(t)} |\psi_0\rangle = e^{k(t)} e^{S(t)} e^{-\tilde{\Sigma}(t)} |\psi_0\rangle , \quad \langle\tilde{\psi}(t)| \equiv e^{-k(t)} \langle\psi_0| e^{\tilde{\Sigma}(t)} e^{-S(t)} . \tag{39}$$

They are the ECCM analogues of the NCCM forms in Eq. (11). The ECCM form for the expectation value $\overline{\mathbb{Q}}(t)$ of an arbitrary physical observable described by the Hermitian operator $q(t)$ to the NCCM form given by Eq. (13) is then given in terms of a double similarity transformation as follows,

$$\langle q(t) \rangle = \overline{\mathbb{Q}}(t) \equiv \langle\psi_0|\mathbb{Q}(t)|\psi_0\rangle ;$$
$$\mathbb{Q}(t) \equiv e^{\tilde{\Sigma}(t)} Q(t) e^{-\tilde{\Sigma}(t)} = e^{\tilde{\Sigma}(t)} e^{-S(t)} q(t) e^{S(t)} e^{-\tilde{\Sigma}(t)} . \tag{40}$$

It is convenient to move from the (linked-cluster) set of c-number coefficients $\{s_I(t), \tilde{s}_I(t)\}$ to a new (and also linked-cluster) ECCM set $\{\sigma_I(t), \tilde{\sigma}_I(t)\}$ belonging to the pair of operators $\{\Sigma(t), \tilde{\Sigma}(t)\}$, where the new linked operator $\Sigma(t)$ is defined as follows,

$$\Sigma(t)|\psi_0\rangle \equiv (\mathbb{1} - |\psi_0\rangle\langle\psi_0|) e^{\tilde{\Sigma}(t)} S(t)|\psi_0\rangle = \sum_{I \neq 0} \sigma_I(t) C_I^+ |\psi_0\rangle . \tag{41}$$

The inverse pair of transformations between the coefficients $\sigma_I(t)$ and $s_I(t)$ are thus given $\forall I \neq 0$ as follows

$$\sigma_I(t) = \langle\psi_0|C_I^- e^{\tilde{\Sigma}(t)} S(t)|\psi_0\rangle , \quad s_I(t) = \langle\psi_0|C_I^- e^{-\tilde{\Sigma}(t)} \Sigma(t)|\psi_0\rangle . \tag{42}$$

The ECCM expectation value functional, $\overline{\mathbb{Q}}(t) = \overline{\mathbb{Q}}[\sigma_I, \tilde{\sigma}_I; t] = \langle q(t) \rangle$, of an observable operator $q(t)$ is now considerably more complicated than its NCCM counterpart $\overline{Q}[s_I, \tilde{s}_I; t]$, due to the presence of the double similarity transformation. A detailed analysis [2,3] has shown, however, that the ECCM counterparts to the NCCM results of Eqs. (16) and (17) are given as follows,

$$\overline{\mathbb{Q}}[\sigma_I, \tilde{\sigma}_I; t] = \sum_{m=0}^{\infty} \frac{1}{m!} \sum_{n=0}^{\infty} \frac{1}{n!} \sum_{J_1 \neq 0} \cdots \sum_{J_m \neq 0} \sum_{K_1 \neq 0} \cdots$$
$$\sum_{K_n \neq 0} \langle J_1, \ldots, J_m | q(t) | K_1, \ldots, K_n \rangle_{\text{ECCM}} \, \tilde{\sigma}_{J_1} \cdots \tilde{\sigma}_{J_m} \sigma_{K_n} \cdots \sigma_{K_1} , \tag{43}$$

where the ECCM matrix elements are now defined as

$$\langle J_1, \ldots, J_m | q(t) | K_1, \ldots, K_n \rangle_{\text{ECCM}} \equiv \langle\psi_0| C_{J_1}^- \cdots C_{J_m}^- \, q(t) \, C_{K_1}^+ \cdots C_{K_n}^+ |\psi_0\rangle_{\mathcal{DL}} . \tag{44}$$

The suffix $\mathcal{DL}$ in Eq. (44) now indicates the ECCM *double linked* structure, which is characterized by the following *two* constraints: (i) from each group of particles characterized by each of the configuration-space indices K_j, the amplitude σ_{K_j} associated with the creation operator $C_{K_j}^+$, must have at least one particle line connected to the operator q (exactly as in the $\mathcal{L}$-linking of the NCCM); and further (ii) for each group of particles characterized by each of the configuration space indices J_k, the amplitude $\tilde{\sigma}_{J_k}$ associated with the destruction operator $C_{J_k}^-$ *either* must have at least one particle line connected to the operator q, *or* there must be connections, by at least one particle line in each case, to at least *two* separate amplitudes σ_{K_j} associated with two different creation operators $C_{K_j}^+$.

The basic ECCM amplitudes $\{\sigma_I, \tilde{\sigma}_I\}$ may thus be viewed as a set of quasilocal classical fields, due to the maximal connectivity feature built into the ECCM. What is meant by quasilocality here is that each of the amplitudes, which now collectively completely characterize the theory and exactly describe the ground ket and bra states, obeys the cluster property in the usual sense of approaching zero in the limit that any one particle or group of particles comprising the many-body cluster becomes far removed from the remainder. In turn this permits applications to, e.g., topological excitations and cases with spontaneous symmetry breaking, that the NCCM would perhaps have difficulties in describing, due to the non-locality of the $\{\tilde{s}_I\}$ amplitudes describing the bra states within the NCCM, which is overcome within the ECCM by the second similarity transformation.

If we now insert the ECCM wave function parametrizations of Eq. (39) into the definition of Eq. (18) of the action functional, and make use of the relationships in Eqs. (41) and (42), it is relatively simple to show that the action now takes the ECCM form,

$$
\begin{aligned}
\mathcal{A} &= \int_{t_0}^{t_1} dt \left\{ -i \sum_{I \neq 0} \left(\frac{d\tilde{\sigma}_I}{dt} \sigma_I \right) - \overline{\mathbb{H}}[\sigma_I, \tilde{\sigma}_I] \right\} \\
&= \int_{t_0}^{t_1} dt \left\{ i \sum_{I \neq 0} \left(\tilde{\sigma}_I \frac{d\sigma_I}{dt} \right) - \overline{\mathbb{H}}[\sigma_I, \tilde{\sigma}_I] \right\}.
\end{aligned}
\tag{45}
$$

The independent (bivariational) stationarity conditions, $\partial \mathcal{A}/\partial \tilde{\sigma}_I = 0 = \partial \mathcal{A}/\partial \sigma_I$, now yield the evolution equations,

$$
i\frac{d\sigma_I}{dt} = \frac{\partial \overline{\mathbb{H}}}{\partial \tilde{\sigma}_I}, \quad -i\frac{d\tilde{\sigma}_I}{dt} = \frac{\partial \overline{\mathbb{H}}}{\partial \sigma_I}; \quad \forall I \neq 0,
\tag{46}
$$

for the ECCM cluster correlation coefficients, which are the the precise counterparts of Eq. (22) in the NCCM case. Equation (46) clearly now shows that the ECCM coefficients σ_I and $\tilde{\sigma}_I$ are again a canonically conjugate pair in exactly the same sense as are s_I and $\tilde{s}_I$ in the NCCM case. As promised earlier, we can now see why the operator S was replaced in the ECCM by the operator Σ via Eq. (41).

It is now evident that the NCCM Eqs. (24) and (25) find their completely analogous ECCM counterparts,

$$
\frac{d\overline{\mathbb{Q}}}{dt} = \frac{\partial \overline{\mathbb{Q}}}{\partial t} + \{\overline{\mathbb{Q}}, \overline{\mathbb{H}}\},
\tag{47}
$$

$$
\{\overline{\mathbb{A}}, \overline{\mathbb{B}}\} \equiv \frac{1}{i} \sum_{I \neq 0} \left(\frac{\partial \overline{\mathbb{A}}}{\partial \sigma_I} \frac{\partial \overline{\mathbb{B}}}{\partial \tilde{\sigma}_I} - \frac{\partial \overline{\mathbb{A}}}{\partial \tilde{\sigma}_I} \frac{\partial \overline{\mathbb{B}}}{\partial \sigma_I} \right).
\tag{48}
$$

The corresponding ECCM expression for the expectation value $\overline{\mathbb{AB}}$ of the product of two ECCM (doubly similarity-transformed) operators is now considerably more complicated

than its NCCM counterpart in Eq. (35). Nevertheless, it can be shown [3] that the expectation value of the commutator of operators $\mathbb{A}$ and $\mathbb{B}$ takes the form

$$\langle [\mathfrak{a}, \mathfrak{b}] \rangle = \overline{[\mathbb{A}, \mathbb{B}]} = \overline{\mathbb{A}\mathbb{B}} - \overline{\mathbb{B}\mathbb{A}} = \mathrm{i}\{\overline{\mathbb{A}}, \overline{\mathbb{B}}\}, \tag{49}$$

within the ECCM, which is the exact analogue of its NCCM counterpart in Eq. (36). It should by now be evident that there are many other analogies between the NCCM and ECCM, which we do not now enumerate further however.

In conclusion, we reiterate that both versions of the CCM can, as we have shown, be formulated in terms of a variational (or, more properly, a bivariational) principle for either the stationary (i.e., time-independent) or time-dependent Schrödinger equations [2,5]. For the stationary (S-CCM) cases of both the NCCM and ECCM the bivariational principle is for the ground-state expectation value functional of the Hamiltonian, while for the time-dependent (TD-CCM) cases it is for the action functional.

2.3 Illustration of stationary aspects of the CCM: the Rabi model

We will elaborate further on the CCM in Sect. 5 where we discuss the physics that lies behind the introduction of non-Hermitian operators, after presenting more of the mathematical framework. For now, however, let us elucidate the use of the CCM in practice via a simple, yet illustrative, example. Among a plethora of possible applications, we choose the Rabi model, an important and archetypal model in quantum optics where it describes a two-level atom (with energy spacing $\hbar\omega_0$) coupled via a dipole interaction (of coupling strength proportional to g) to a single mode of a quantized electromagnetic radiation field (with frequency ω) [25]. In units where $\hbar = 1$, the model is defined by the Hamiltonian,

$$\mathfrak{h} = \frac{1}{2}\omega_0 \sigma^z + \omega b^\dagger b + g\left(\sigma^+ + \sigma^-\right)\left(b^\dagger + b\right), \tag{50}$$

in terms of pseudo-spins

$$\sigma^z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \quad \sigma^+ = \begin{pmatrix} 0 & 2 \\ 0 & 0 \end{pmatrix}, \quad \sigma^- = \begin{pmatrix} 0 & 0 \\ 2 & 0 \end{pmatrix}, \tag{51}$$

related to the conventional Pauli matrices,

$$\sigma^x = \frac{1}{2}\left(\sigma^+ + \sigma^-\right), \quad \sigma^y = \frac{\mathrm{i}}{2}\left(\sigma^- - \sigma^+\right). \tag{52}$$

The field mode is described in terms of the annihilation and creation operators, b and $b^\dagger$, respectively, which obey the usual bosonic commutation relation,

$$\left[b, b^\dagger\right] = \mathbb{1}. \tag{53}$$

Within the context of nuclear magnetic resonance, the model also mimics a spin interacting with a field of phonons [26]. A close relationship of the model also exists to the static Lee model of nuclear interaction [27].

From our present viewpoint the Hamiltonian of Eq. (50) is suitable not only as a rather transparent model of physical reality but also as a useful example to illustrate the applicability and efficiency of the standard NCCM approach (and see Refs. [28,29] for more details). A convenient choice of reference state for this model is now $|\psi_0\rangle = |0\rangle|\downarrow\rangle$, which is just the ground state of the system for $g = 0$, assuming $\omega_0 > 0$ (viz. an empty field mode and an unexcited atom), in a notation where the first ket refers to zero bosons in the occupation number representation and the second to the lower state of the two-level atom in an obvious

pseudo-spin representation with the spin quantized in the z-direction. For example, the generic NCCM correlation operators of Eq. (12) can now be written in the following specific forms,

$$S = S_1 + S_2 \,; \quad S_1 = \sum_{n=1}^{\infty} s_n^{(1)} (n!)^{-1/2} (b^\dagger)^n \,,$$

$$S_2 = \sum_{n=1}^{\infty} s_n^{(2)} [4(n-1)!]^{-1/2} (b^\dagger)^{n-1} \sigma^+ \,,$$

(54a)

$$\tilde{S} = \mathbb{1} + \tilde{S}_1 + \tilde{S}_2 \,; \quad \tilde{S}_1 = \sum_{n=1}^{\infty} \tilde{s}_n^{(1)} (n!)^{-1/2} b^n \,,$$

$$\tilde{S}_2 = \sum_{n=1}^{\infty} \tilde{s}_n^{(2)} [4(n-1)!]^{-1/2} b^{n-1} \sigma^- \,.$$

(54b)

The only approximation that is now made is to truncate the sums in Eqs. (54a) and (54b) at the term with $n = N$, giving the so-called SUB-N approximation, in which all the coefficients $s_n^{(i)}$ and $\tilde{s}_n^{(i)}$, $i = 1, 2$, are set to zero $\forall n > N$.

In the stationary version of the NCCM, one may now readily evaluate the ground-state expectation value, $\langle \mathfrak{q} \rangle = \overline{Q} = \overline{Q}[s_I, \tilde{s}_I]$ of any physical observable $\mathfrak{q}$ for the Rabi model, as described in Sect. 2.1. For example, the ground-state energy, $E = \langle \mathfrak{h} \rangle$, has been so calculated at various NCCM SUB-N levels of approximation in Ref. [28], to which the interested reader is referred for further details. We note only that with the above choices of reference state and cluster operators the NCCM was found to yield a (probably spurious) phase transition at a value $g \rightarrow g_c \approx 0.665$ of the coupling constant, which signaled a breakdown of the (convergence of the) calculation for values $g > g_c$, which is precisely the region where the ground state becomes nearly degenerate in energy with the first excited state of the system [30]. Still, the method provided excellent results for E in the region $g < g_c$. We defer further discussion of applications of the TD-CCM to this and other systems to Sect. 6.

3 Excited states and non-Hermitian reformulations of conventional quantum mechanics

We shall consider the question of how to construct excited states and the excitation spectrum of a quantum many-body system within the CCM later in Sect. 7. However, we note now that whenever one tries to move beyond the CCM-based precise evaluations of the ground-state characteristics of a generic (i.e., not even necessarily just many-body) quantum system, one may encounter a number of new, and sometimes unexpected, methodical challenges. At an initial level of approach it appears that one must find a way of making any CCM-inspired explicit construction of an optimal Dyson map $\Omega = \exp S$ of Eq. (4) sufficiently less reference-dependent. For example, in the nuclear-physics IBM-related setting of Ref. [31], this appeared to be a decisive technical obstacle.

The essence of the difficulty lies in the fact that the descriptive ambitions of the IBM constructions involved not only the single ground state but also whole multiplets of the low-lying excited states. In this setting, a decisive amendment of the variational results (see the thorough review and mathematical clarification and explanation of Scholtz et al. [32]) only appeared after a return of attention to the older Dyson's papers on ferromagnetism [33,34]

in which calculational success was essentially based on the use of a *non-unitary* operator Ω in Eq. (2).

The latter idea has later been identified as yielding a nontrivial form for the auxiliary operator product $\Omega^\dagger \Omega$ which is henceforth called the *metric operator* of the physical Hilbert space,

$$\Omega^\dagger \Omega \equiv \Theta \neq \mathbb{1} \,, \tag{55}$$

where $\mathbb{1}$ is again the identity operator. During the subsequent developments of the field different authors succeeded in finding techniques circumventing the obstacles emerging due to the nontrivial nature of the metric (i.e., that it is not simply the identity operator), which is not encountered in conventional Hermitian quantum mechanics.

The computational economy of the Hermitian Schrödinger-picture (SP) formulation of quantum mechanics [35] is very persuasive. It is just this aspect of the formulation that explains its popularity and success in many branches of quantum physics and quantum chemistry. Nevertheless, several existing technical limitations of the conventional SP description of quantum mechanics have almost always forced its users to search for amendments. In this context a short letter by Bender and Boettcher [36] proved to be very influential in returning attention to the less usual but fully admissible possibility of non-Hermitian representations of observables as promoted, a few years earlier, in Ref. [32]. The latter paper itself actually recalled the older idea of mapping certain Hermitian fermion operators onto simpler non-Hermitian boson operators by means of the generalized Dyson mapping [37], with all of these developments being precisely the motivation behind the IBM technique itself [7–9].

Such a "crypto-Hermitian" amendment (or perhaps, better, extension) of our understanding of quantum theory has, at present, multiple parallels and continuations [14]. The resulting, truly deep, theoretical reconsideration of the first principles of quantum theory has now become widely accepted by a broad community of physicists. The impact of the idea may nowadays be detected even beyond the domain of quantum theory [38]. Still, its origins may be dated back to the studies of certain truly complicated many-fermion quantum systems. It was, in fact, Dyson [33,34] (and, independently, Maleev [39]) who proposed, more than 60 years ago, and mainly for the purely practical purposes of variational calculations, a key idea lying in the (formally reversible) *non-unitary* mapping of wave functions as in Eq. (2).

The reader should be aware at this point that up till now we have not precisely defined the term "Hermitian" on the mathematical level. In general, one would need to distinguish with care such alternative concepts related to the term "Hermitian" as "symmetric", "self-adjoint" (on a specified domain), and "essentially self-adjoint" (with a well-defined core). However, in most of the prospective applications that we have in mind we work with a finite-dimensional matrix form of the so-called "Hermitian" operator, in which case there is no longer any need for such mathematical precision. Marginally, let us note here that, even in the infinite-dimensional and non-matrix models, the essence of many related apparent paradoxes can be identified as lying in the fact that the physical Hilbert space is exclusively presented via its representation in $\mathcal{H}_{[\text{unphysical}]}^{(\text{user–friendly})}$. Thus, the clarification of the Hermiticity/non-Hermiticity misunderstandings becomes simple when one consequently stays in the latter space and characterizes the switch to $\mathcal{H}_{[\text{physical}]}^{(\text{final})}$ by the mere change of the inner product (and the interested reader can find further useful comments on this trick in Ref. [14]).
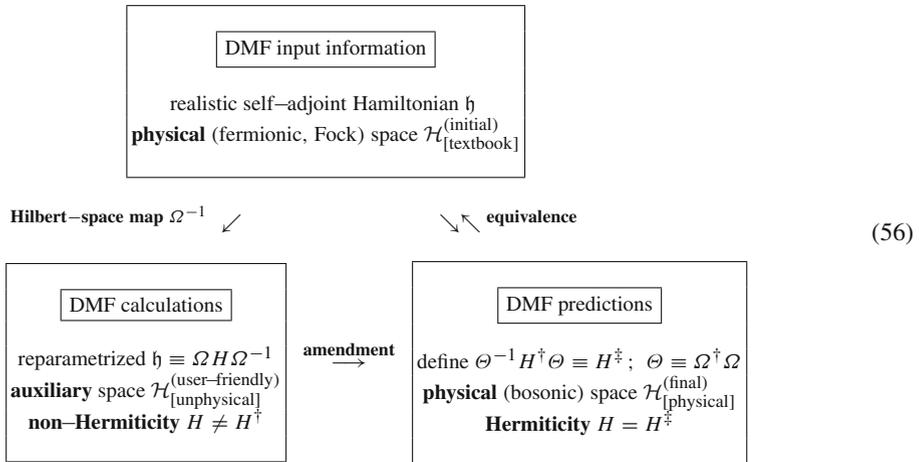
Due to the latter trick, phenomenological Hamiltonians may be, admittedly, manifestly non-Hermitian in a preselected and, presumably, just unphysical, auxiliary Hilbert space $\mathcal{H}_{[\text{unphysical}]}^{(\text{user–friendly})}$. As a concrete example let us recall the most popular, ordinary differential, upper-case Hamiltonian $H^{(\text{imaginary cubic})} = -\frac{\mathrm{d}^2}{\mathrm{d}x^2} + \mathrm{i}x^3$, which is $\mathcal{PT}$-symmetric [13,36] but

manifestly non-Hermitian in $\mathcal{H}^{\text{(user–friendly)}}_{\text{[unphysical]}} = L^2(\mathbb{R})$. After an appropriate amendment of the inner product, according to Bender [13], the underlying quantum system $\mathcal{S}$ may be assigned its conventional quantum probabilistic unitary-evolution interpretation via the reconstruction of the physical Hermitian conjugation [c.f., the "physical" conjugation $H \to H^{\ddagger} \equiv \Theta^{-1} H^{\dagger} \Theta$ in place of the conventional, friendlier but unphysical, conjugation $H \to H^{\dagger}$.

There exist many interesting aspects of the model described by $H^{\text{(imaginary cubic)}}$ and by its various alternatives, which are explained and discussed in, e.g., the reviews presented in Refs. [12–14]. For all of them the underlying probabilistic interpretation of the quantum systems is based on the innovative use of non-Hermitian Hamiltonian avatars H with real energy eigenvalue spectra. Almost without exception, all of these examples are presented, in the current literature, in the framework of what we will call here the generalized (i.e., "non-Hermitian") Schrödinger-picture formalism. In its stationary case we will call it, for the sake of definiteness, the Dyson–Maleev formalism (DMF), for a particularly extensive review of the generalized forms of which we may particularly recommend Ref. [37].

Once one manages to achieve at least a reasonable degree of reference-independence of Ω, a suitable combination of the CCM mathematics with IBM physics could open new construction horizons. Indeed, in the strictly stationary case, i.e., in the case with property $\Omega(t) = \Omega(0)$, $\forall t$, there exists an intimate connection and correspondence between the generality (i.e., non-unitarity) of Ω, the non-Hermiticity of the avatars H of the Hamiltonians given by Eq. (3) and the bivariational nature of the CCM recipes, as we discussed in our previous paper [1].

The DMF approach may be perceived as one of the standard numerical algorithms, which transfers the description of the states from the traditional (i.e., often, fermionic, Fock) Hilbert space $\mathcal{H}^{\text{(initial)}}_{\text{(DMF)}} = \mathcal{H}^{\text{(fermionic)}}_{\text{(DMF)}}$ of wave functions ψ to its *formally non-equivalent* (i.e., often, effective, bosonic) Hilbert space $\mathcal{H}^{\text{(unphysical)}}_{\text{(DMF)}} = \mathcal{H}^{\text{(bosonic)}}_{\text{(DMF)}}$ of wave functions ψ_0. The resulting gain in flexibility is remarkable, being broadly appreciated and widely applied [7–9,37]. In the context of the DMF theory the non-equivalence of the two Hilbert spaces $\mathcal{H}^{\text{(fermionic)}}_{\text{(DMF)}}$ and $\mathcal{H}^{\text{(bosonic)}}_{\text{(DMF)}}$ proved inessential. In the latter space one can always amend the inner product in such a way that the resulting new, third Hilbert space $\mathcal{H}^{\text{(final)}}_{\text{(DMF)}}$ becomes eligible to play the role of the ultimate Dyson-Maleev physical Hilbert space [31,33,37,39–43]. For this reason the predictions of the DMF approach are essentially identical to those of the conventional Schrödinger picture, provided only that the third, final space is, by construction, assumed unitarily equivalent to the initial one, $\mathcal{H}^{\text{(final)}} \sim \mathcal{H}^{\text{(initial)}}$. For this reason the key features of the stationary DMF scheme (typically, in its nuclear-physics IBM implementations) remain transparent. Its structure may be summarized by the following compact illustrative flowchart diagram,

$$
\begin{array}{c}
\boxed{\text{DMF input information}} \\[4pt]
\text{realistic self–adjoint Hamiltonian } \mathfrak{h} \\
\textbf{physical} \text{ (fermionic, Fock) space } \mathcal{H}^{(\text{initial})}_{[\text{textbook}]}
\end{array}
$$

$$
\textbf{Hilbert–space map } \Omega^{-1} \; \swarrow \qquad\qquad\qquad \searrow\nwarrow \textbf{ equivalence} \tag{56}
$$

$$
\begin{array}{c}
\boxed{\text{DMF calculations}} \\[4pt]
\text{reparametrized } \mathfrak{h} \equiv \Omega H \Omega^{-1} \\
\textbf{auxiliary} \text{ space } \mathcal{H}^{(\text{user–friendly})}_{[\text{unphysical}]} \\
\textbf{non–Hermiticity } H \neq H^{\dagger}
\end{array}
\qquad
\overset{\textbf{amendment}}{\longrightarrow}
\qquad
\begin{array}{c}
\boxed{\text{DMF predictions}} \\[4pt]
\text{define } \Theta^{-1} H^{\dagger} \Theta \equiv H^{\ddagger}; \; \Theta \equiv \Omega^{\dagger}\Omega \\
\textbf{physical} \text{ (bosonic) space } \mathcal{H}^{(\text{final})}_{[\text{physical}]} \\
\textbf{Hermiticity } H = H^{\ddagger}
\end{array}
$$

One of the most remarkable consequences of the non-unitarity of the mapping Ω, seen in such a diagram lies in the *coexistence* of the Hermiticity and non-Hermiticity properties of *the same* upper-case operator H, depending on which Hilbert space one is considering. In the stationary setting the above-mentioned operator H represents an observable quantity, *despite* being non-Hermitian (in the sense that $H \neq H^{\dagger}$) in $\mathcal{H}^{(\text{user–friendly})}_{[\text{unphysical}]}$, precisely *because* it is self-adjoint (in the sense that $H = H^{\ddagger}$) in $\mathcal{H}^{(\text{final})}_{[\text{physical}]}$.

3.1 Transition to non-stationary quantum systems

Our present study was inspired by the recent progress in the development of what could be called reference-independent IBM-like theories [11,44–47]. The message of our present paper should be seen in the transfer of our current understanding of the merits of the mappings of Eq. (2) from the IBM-related context into the bivariational constructive CCM strategies. The NHIP formulation of quantum mechanics will be used, in such an application, in a slightly narrower sense, being reserved to cover only the picture of reality with the non-stationarity property,

$$
\Omega_{(\text{NHIP})} = \Omega_{(\text{NHIP})}(t) .
$$

According to the first consistent introduction of the full-fledged non-stationary NHIP formalism in Ref. [44], its basic idea may be perceived as a time-dependent extension of the old IBM-like variational recipe. While its innovated form is definitely more flexible, it is undoubtedly also much more complicated technically [45]. For this reason it is, therefore, perhaps not too surprising that the TD-CCM/NHIP relationship has not yet been studied. It is precisely this omission that we aim to remedy here. This technical complexity also probably explains why only a relatively few realistic applications of several alternative implementations of the NHIP ideas themselves may yet be found in the current literature [45,47–56].

Since the birth of quantum theory in its Heisenberg-picture (HP) formulation [57] and, less than a year later, in its Schrödinger-picture (SP) formulation [35], those attempting to apply the theory have always needed to resolve the conflict between the more intuitive nature of the HP quantization of observables and the maximal economy of the transfer of attention to the wave functions in the SP approach. A partial relief of this tension came, later, with the invention of the more universal interaction-picture (IP) (alias the Dirac-picture) formalism

Table 1 Conventional Hermitian-generator descriptions of quantum dynamics

Picture	Observables $\mathfrak{q}(t)$	State vectors $\psi(t)$
HP	Evolving	Constant
SP	Constant	Evolving
IP	Evolving	Evolving

from which the SP and HP descriptions of quantum dynamics could have been deduced as two separate special limiting cases. An enhanced flexibility of the ensuing language then also gave rise to the well-known successes of the manifold IP applications (and predictions) in practice, especially in the context of quantum field theory and quantum many-body theory [58,59].

In Table 1 we present a comparison of the HP, SP and IP "strictly Hermitian" descriptions of unitary (i.e., stable) quantum evolution. As a comment on the table we might emphasize that the same physics is described by the *single* operator evolution equation in the HP formulation, and by the *single* ket-vector evolution equation in the SP formulation, as well as by a *pair* of evolution equations in the IP formulation. For a compensation of the seeming disadvantage of the doubling of the number of evolution equations in the IP formalism, we note again that the latter IP picture contains both the former (HP and SP) ones as special limiting cases.

The ultimate choice between the HP, SP and IP (or, indeed, many other [60]) model-building strategies depends, first of all, on the actual form of our specification of the quantum system in question. For this reason, most standard textbooks usually prefer the SP language, only adding the HP and IP analyses of quantum dynamics at the later stages of explanation. This makes the SP-based specification of quantum dynamics less intuitive but shorter, based on the rather formal introduction of a "physical" Hilbert space $\mathcal{H}^{(\text{initial})}$ and of a suitable self-adjoint "Hamiltonian" $\mathfrak{h} = \mathfrak{h}^{\dagger}$ defined within that space. Many researchers prefer the use of the SP language in practice, since it requires, in addition, a maximally realistic origin for, and "derivation" of, the latter Hamiltonian operator, which is typically found, e.g., via a "quantization" of its suitable classical-physics counterpart.

3.2 Non-Hermitian versions of the Heisenberg and Dirac pictures

The key to the extension of the validity of the IBM-type pattern beyond its stationary DMF version of Eq. (56) has been found in Ref. [44]. First of all, the removal of the existing theoretical obstacles and objections (and see, e.g., Ref. [61]) required a refinement of the terminology. In Ref. [44] it has been emphasized that the initial and observable physical Hamiltonian $\mathfrak{h}(t)$ (defined in $\mathcal{H}^{(\text{initial})}_{[\text{textbook}]}$; in general it may be time-dependent) merely becomes replaced, as in Eq. (58), by its upper-case isospectral *non-stationary* avatar,

$$H(t) \equiv \Omega^{-1}(t)\mathfrak{h}(t)\Omega(t), \tag{57}$$

which is non-Hermitian in $\mathcal{H}^{(\text{user-friendly})}_{[\text{unphysical}]}$ but Hermitian in $\mathcal{H}^{(\text{final})}_{[\text{physical}]}$ [i.e., in the sense that $H = H^{\ddagger}$, where $H^{\ddagger} \equiv \Theta^{-1} H^{\dagger} \Theta$, as in the flowchart of Eq. (56)]. For this reason, both of the operators $\mathfrak{h}(t)$ and $H(t)$ represent an instantaneous energy, i.e., the same observable physical quantity. Clearly, Eq. (57) is simply the time-dependent counterpart of its stationary equivalent in Eq. (3). However, the clarification of the *dynamical role* of the two operators $\mathfrak{h}(t)$ and $H(t)$ in Eq. (57) has turned out to be much less straightforward. In the literature, the process of this clarification was both lengthy and tedious [44,61–66]. Fortunately, at the end of this process in 2009 (c.f., Ref. [11] and some later addenda in Refs. [52–54]) the eventual

outcome has transpired to be both relatively elementary and transparent, as we now briefly explain.

Its brief summary may start from a return to Table 1, which reminds us that even in the conventional Hermitian SP setting the SP $\to$ HP transition may be perceived as mediated by a mapping of the form of Eq. (2), but in which the operator Ω would be unitary but manifestly time-dependent. In 2007, the feasibility of the extension of the SP $\leftrightarrow$ HP correspondence to non-Hermitian cases was opposed by Mostafazadeh [14,61,63,66]. Fortunately, the apparently insurmountable obstacles and obstructions that were initially raised against the free applicability of the non-stationarity postulate,

$$\Omega_{\text{(NHHP)}} = \Omega_{\text{(NHHP)}}(t) \,,$$

thereafter appeared in essence to be of a purely terminological nature [44,62,64,65,67,68]. As a consequence, the transition to the generalized "non-Hermitian" HP (viz. the NHHP) was eventually formulated definitively in Ref. [46]. Soon thereafter it was also found to be both feasible and useful in practice in some specific applications [69].

Once we are given a lower-case SP operator q representing an arbitrary observable quantity, the only relevant task for theorists is a prediction of the results of experiments based on the evaluation of its expectation value. This means that we have to evaluate the quantity

$$\langle\!\langle \psi(t)|Q(t)|\psi(t)\rangle \,.$$

The precise meaning of the ket state $|\psi(t)\rangle$ and of the bra (or, rather, brabra) state $\langle\!\langle \psi(t)|$, are to be specified of course (see Sect. 4.1). The upper-case symbol $Q(t)$ just represents here the operator (isospectral to q), which is defined in the space $\mathcal{H}^{\text{(user–friendly)}}_{\text{[unphysical]}}$ via a similarity transformation

$$Q(t) \equiv \Omega^{-1}(t)\mathfrak{q}\Omega(t) \,, \tag{58}$$

in complete analogy to its NCCM counterpart in Eq. (14a). The overall theoretical flowchart then has the following compact form,

$$\tag{59}$$
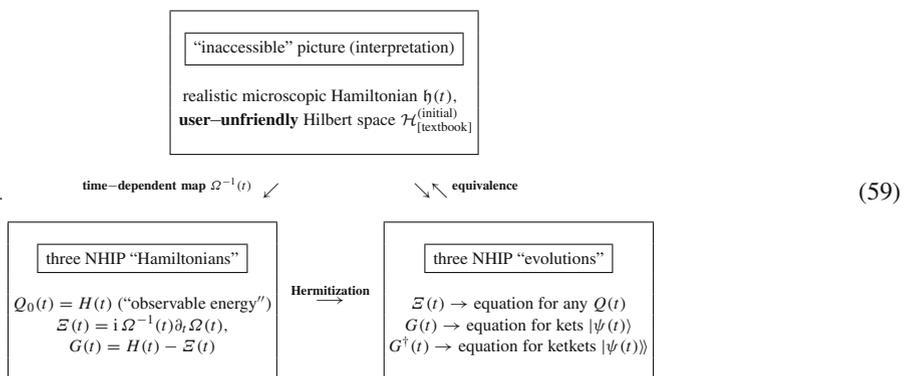
The precise meaning and definitions of the operators and state vectors in Eq. (59) is given in Sect. 4. On this basis we may expect that the use of the alternative formulations of the dynamical equations will not hide their one-to-one correspondences with those in the Hilbert space $\mathcal{H}^{\text{(initial)}}_{\text{[textbook]}}$ of the topmost-box in the diagram comprising Eq. (59).

4 Non-Hermitian versions of dynamical evolution equations

Curiously enough, the above-outlined NHHP formalism is "quasi-stationary" because the HP metric itself remains time-independent [45,46],

$$\Theta_{(HP)}(t) = \Theta_{(HP)}(0) \,. \tag{60}$$

As a consequence, it was necessary to move beyond the constraint (60) (c.f., Ref. [47]). The current state of the art is summarized in Table 2 in which the third "non-Hermitian", fully general formalism of Refs. [44,47] is now assigned the abbreviation NHIP. Clearly, Table 2 is just the general counterpart in our non-Hermitian context of the earlier Table 1 that pertains to the conventional Hermitian-generator description of unitary evolution.

4.1 Recommended notation conventions

In the most general NHIP context the use of the non-stationary, Dyson-motivated Ansatz of Eq. (2) seems to open a Pandora's box of thorny problems. First of all, once we accept the fact that $\Omega = \Omega(t)$ is a map which inter-relates a triplet of Hilbert spaces, we find that the notation is insufficient and/or incomplete. Thus, first of all, it does not inform us that such a map connects the initial-reference ket $\psi_0 \in \mathcal{H}_{[\text{textbook}]}^{(\text{initial})}$ and the final-reference ket $\psi \in \mathcal{H}_{[\text{unphysical}]}^{(\text{user–friendly})}$, which may then itself be re-read, alternatively, as the correct physical ket $\psi \in \mathcal{H}_{[\text{physical}]}^{(\text{final})}$. Secondly, one would also like to avoid using the subscript 0 in ψ_0 because the symbols ψ and ψ_0 refer, in fact, to *the same* quantum state in the NHIP representation.

Both of these inconsistencies of notation were successfully removed in Ref. [11], in which it was shown how all of the unnecessary repetitions of the, otherwise necessary, explanatory comments may be circumvented by using the following three simple amendments of the standard Dirac notation for state vectors, viz. by using the triplet of replacements

$$\psi \to |\psi \succ \,, \quad \psi_0 \to |\psi\rangle \,, \quad \Theta\,\psi_0 \to |\psi\rangle\!\rangle \equiv \Theta\,|\psi\rangle \,. \tag{61}$$

The defining relation between the ket state $|\psi(t)\rangle$ and the ketket state $|\psi(t)\rangle\!\rangle$ in Eq. (61) validates our earlier assertion in Eq. (60) that the HP metric operator $\Theta_{(HP)}$ is stationary since, by definition (and see Table 2), neither of these states evolves in time in an HP formalism.

Continuing with the exposition of our recommended notation convention in the three-Hilbert-space approach, we note that the NHIP version of our fundamental Ansatz of Eq. (2), viz.

$$|\psi(t)\succ \,= \Omega(t)\,|\psi(t)\rangle \,, \tag{62}$$

in terms of the ket state $|\psi(t)\rangle$, may equivalently be re-written as

$$|\psi(t)\succ \,= \left[\Omega^\dagger(t)\right]^{-1}|\psi(t)\rangle\!\rangle \,, \tag{63}$$

Table 2 Unitary evolution in non-Hermitian pictures	Generalized picture type	Evolution equations for		
		$Q(t)$	$|\psi(t)\rangle$	$|\psi(t)\rangle\!\rangle$
	Schrödinger, NHSP ≡ DMF	–	Yes	Yes
	Heisenberg, NHHP	Yes	–	–
	(Dirac) interaction, NHIP	Yes	Yes	Yes

in terms of the ketket state $|\psi(t)\rangle\rangle$. The unphysical nature of the auxiliary Hilbert space is now evident because the mean value of the operator representing a self-adjoint (textbook) lower-case observable [say, $\mathfrak{q}(t)$] becomes different from that of its upper-case auxiliary-space counterpart,

$$\prec\psi(t)|\mathfrak{q}(t)|\psi(t)\succ \ = \langle\psi(t)|\Omega^{\dagger}(t)\mathfrak{q}(t)\Omega(t)|\psi(t)\rangle \tag{64}$$

$$= \langle\psi(t)|\Theta(t)Q(t)|\psi(t)\rangle \neq \langle\psi(t)|Q(t)|\psi(t)\rangle. \tag{65}$$

In the derivation we have employed the definition of $Q(t)$ given in Eq. (58). Using our notations we thus also reveal the correct physical status of the final Hilbert space $\mathcal{H}_{[\text{physical}]}^{(\text{final})}$, since Eqs. (64) and (65) clearly display the *equality* of the *measurable* quantities in the two respective Hilbert spaces $\mathcal{H}_{[\text{textbook}]}^{(\text{initial})}$ and $\mathcal{H}_{[\text{physical}]}^{(\text{final})}$,

$$\prec\psi(t)|\mathfrak{q}(t)|\psi(t)\succ \ = \langle\langle\psi(t)|Q(t)|\psi(t)\rangle. \tag{66}$$

The required matrix element in the latter space [i.e., that on the right-hand side of Eq. (66)] is precisely the one that we introduced earlier in the discussion in Sect. 3.2.

We never need to leave the auxiliary Hilbert space. One can say even more: thus, any physical quantum state can be characterized by ket $|\psi(t)\rangle$ and metric $\Theta(t)$ or, much more economically, by the pair comprising ket $|\psi(t)\rangle$ and ketket $|\psi(t)\rangle\rangle$. Similarly, one can say that any physical observable can be characterized by its "hiddenly-Hermitian" operator $Q(t)$ and metric $\Theta(t)$ or, without an explicit use of the metric, by the pair of operators $Q(t)$ and $Q^{\dagger}(t)$, mutually connected by the metric,

$$Q^{\dagger}(t)\,\Theta(t) = \Theta(t)\,Q(t). \tag{67}$$

Equation (67), which is easily derived from the definitions of $\Theta(t)$ and $Q(t)$ in Eqs. (55) and (58), respectively, is just the so-called hidden-Hermiticity (alias quasi-Hermiticity) relation [32,70] for an operator $Q(t)$ in the NHIP formalism that belongs to a physical observable. It is, of course, completely equivalent to the relation

$$\Theta^{-1}(t)Q^{\dagger}(t)\Theta(t) \equiv Q^{\ddagger}(t) = Q(t), \tag{68}$$

which provides simply the obvious generalization of the definition of $H^{\ddagger}$ in the flowchart of Eq. (56). It is worth noting that the operator Θ itself is *both* Hermitian in the ordinary sense *and* quasi-Hermitian in the sense of Eq. (68). More generally, so is any operator that may be expressed as an arbitrary power series in Θ with real-valued coefficients.

As an aside here, we can now directly compare the present NHIP formalism with the earlier NCCM description. Thus, in the NCCM the reference (or model) state ψ_0 is assumed to be *stationary* (i.e., time-independent). By comparison of Eqs. (13) and (14a) with Eqs. (64) and (65,), we also see that the NCCM operator $\tilde{S}(t)$ is (up to a multiplicative normalization constant) precisely equal to the NHIP metric operator, viz. $\tilde{S}(t) = \Theta(t)/\langle\psi(t)|\Theta(t)|\psi(t)\rangle$, in our newly recommended NHIP notation.

4.2 Evolution equations for states

In the light of the definition, given by Eq. (57), of the isospectral non-Hermitian partner $H(t)$ of the textbook Hamiltonian $\mathfrak{h}$, one can now claim that the upper-case operator $H(t)$ is, indeed, quasi-Hermitian,

$$H^{\dagger}(t)\,\Theta(t) = \Theta(t)\,H(t), \tag{69}$$

in the sense of Refs. [32,70,71], and in accord with Eq. (67). Such an observable for the Hamiltonian is now to be interpreted as an instantaneous total energy. Its observability status reflects the observability of its (manifestly Hermitian in the usual sense) isospectral partner $\mathfrak{h} = \mathfrak{h}^{\dagger}$.

Several authors (ranging from Bíla [50,51] up to his most recent followers [67]) decided to re-assign the status of Hamiltonian to another operator. The explanation of this slightly surprising decision is purely terminological. A detailed disentanglement of the puzzle has been given recently [47], which we now briefly summarize since it is very pertinent to our own further developments here. It starts from the conventional initial-space SP evolution equation given by Eq. (1), now rewritten in our new notation of Eq. (61) as

$$i\partial_t |\psi(t)\succ = \mathfrak{h} \, |\psi(t)\succ \ , \tag{70}$$

and thence from its replacement by the preconditioned NHIP alternative defined in $\mathcal{H}_{[\text{unphysical}]}^{(\text{user--friendly})}$. The latter, equivalent Schrödinger-like evolution equation for ket states $|\psi(t)\rangle$,

$$i\partial_t |\psi(t)\rangle = G(t) \, |\psi(t)\rangle \, ; \tag{71}$$

$$G(t) \equiv H(t) - \varXi(t) \, , \quad \varXi(t) \equiv i\Omega^{-1}(t) \, [\partial_t \Omega(t)] \, . \tag{72}$$

is easily derived from Eq. (62). It contains, naturally, the generator of evolution which is composed of the energy operator $H(t)$ in combination with the so-called Coriolis operator $\varXi(t)$ [45], as we observe explicitly in Eq. (72). For this reason, the re-assignment of the name of the Hamiltonian from $H(t)$ to the newly constructed operator $G(t)$, as has been suggested by several authors (see, e.g., Refs. [50,51,67]) as mentioned above, is, in our view, both misleading and unfortunate.

In our notation any given quantum state is labeled by *the same* Greek letter (say, ψ). Hence, we conclude that once we are describing the state in terms of a *pair* of independent vectors $|\psi(t)\rangle$ and $|\psi(t)\rangle\rangle$, we may utilize Eq. (61), which gives the relationship between them, together with Eqs. (69), (71), and (72), to derive the complementary, second, *independent* evolution law for ketket states $|\psi(t)\rangle\rangle$,

$$i\partial_t |\psi(t)\rangle\rangle = G^{\dagger}(t) \, |\psi(t)\rangle\rangle \, . \tag{73}$$

In this equation, nobody has, as yet, further re-assigned the traditional name of the Hamiltonian to $G^{\dagger}(t)$. Thus, for our current purposes we will reserve the name of an "evolution generator" for *both* of the operators $G(t)$ and $G^{\dagger}(t)$.

4.3 Evolution equations for observables

Given the NHIP Coriolis operator and the initial (i.e., at time $t = 0$) values of the metric $\Theta(0)$ and of an arbitrary observable operator $Q(0)$, such that

$$Q^{\dagger}(0)\Theta(0) = \Theta(0)Q(0) \, , \tag{74}$$

we may reconstruct the full time-dependence of $Q(t)$ via the following NHIP version of the Heisenberg equation,

$$i\partial_t Q(t) = Q(t)\varXi(t) - \varXi(t)Q(t) \equiv [Q(t), \varXi(t)] \, . \tag{75}$$

We may also work with its conjugate version for complement $Q^{\dagger}(t)$,

$$i\partial_t Q^{\dagger}(t) = [Q^{\dagger}(t), \varXi^{\dagger}(t)] \, . \tag{76}$$

In the light of Eqs. (67), (75) and (76), the initial condition of Eq. (74) at time $t = 0$ will guarantee the observability status of $Q(t)$ at all times, as required of course, as we now show explicitly. In particular, if we define the operator,

$$\mathcal{Z}(t) \equiv Q^\dagger(t)\Theta(t) - \Theta(t)Q(t) \,,$$

which is *not* an observable, and hence does *not* evolve as given by Eq. (75), we may use Eqs. (75) and (76), together with the definition of $\Theta(t)$ in Eq. (55), to show directly that its actual evolution equation is instead given by

$$\mathrm{i}\partial_t \mathcal{Z}(t) = \mathcal{Z}(t)\Xi(t) - \Xi^\dagger(t)\mathcal{Z}(t) \,,$$

which clearly has the solution $\mathcal{Z}(t) = 0$ for all times t under the initial condition $\mathcal{Z}(0) = 0$, as given by Eq. (74). Indeed, straightforward differentiation of the definition of $Q(t)$ in Eq. (58) (and of its conjugate) with respect to time yields immediately (the two commutator-containing) Eqs. (75) and (76). Naturally, we assume in so doing that the inaccessible SP operator q does not vary with time. We do not consider further here the strongly anomalous case of a manifestly time-dependent operator, q = q(t), except to note that it has also been discussed in Ref. [46].

Let us now return to Eq. (71) [skipping an analogous analysis of its adjoint partner in Eq. (73)] and let us notice that it contains the operator $G(t)$ of Eq. (72) which is not only non-Hermitian but even non-quasi-Hermitian in our working Hilbert space $\mathcal{H}_{[\text{unphysical}]}^{(\text{user–friendly})}$. It is worth adding that it plays not only the role of the generator of the evolution of the state-vector kets, as exhibited in Eq. (71), but also the role of the generator of the evolution of the observable instantaneous energy. It is easy to verify the validity of the evolution equation

$$\mathrm{i}\partial_t H(t) = [G(t), H(t)] = [H(t), \Xi(t)] \,, \tag{77}$$

where the last equality, which follows simply from the definition of $G(t)$ in Eq. (72), is thus completely compatible with Eq. (75). Equation (77) thus determines the Hamiltonian $H(t)$ from any initial value $H(0)$ such that $H^\dagger(0)\Theta(0) = \Theta(0)H(0)$.

Even in the case of strictly unitary evolution and even in the HP subcase of the general (and entirely methodical) NHIP scheme, as outlined above, both of the operators $\Xi(t)$ and $\Xi^\dagger(t)$ should properly be called Coriolis-force potentials (or, more simply, Coriolis terms) rather than Hamiltonians. The name Hamiltonian should, for reasons thus outlined, remains consistently restricted only to the quasi-Hermitian observable $H(t)$ and/or, whenever needed, to its conjugate operator $H^\dagger(t)$. This is only reinforced by the fact that none of the other, rejected candidates (from those introduced above) for possible promotion to Hamiltonian status even need to have a real eigenvalue spectrum in general, as may rather easily be illustrated.

Thus, for example, we may readily prove the relation,

$$\mathrm{i}\Omega(t)\left[\Xi^\dagger(t) - \Xi(t)\right]\Omega^\dagger(t) = \Omega(t)\partial_t\Omega^\dagger(t) + [\partial_t\Omega(t)]\Omega^\dagger(t) = \partial_t\left[\Omega(t)\Omega^\dagger(t)\right] \,,$$

simply by making use of the definition of $\Xi(t)$ from Eq. (72). This relation implies that the (generally) non-Hermitian Coriolis operator $\Xi(t)$ has real eigenvalues [i.e., when it becomes Hermitian, $\Xi^\dagger(t) = \Xi(t)$] only in the special case in which the self-adjoint image $\theta(t)$ in the original space $\mathcal{H}_{[\text{textbook}]}^{(\text{initial})}$ of the self-adjoint Hilbert-space metric $\Theta(t)$ in the final space $\mathcal{H}_{[\text{physical}]}^{(\text{final})}$, defined, exactly as in the general case of Eq. (58), as

$$\theta(t) \equiv \Omega(t)\Theta(t)\Omega^{-1}(t) = \Omega(t)\Omega^\dagger(t) = \theta^\dagger(t) \,,$$

remains time-independent.

5 Physics behind non-stationary non-Hermitian operators

The initial motivation of our interest in the mutual relationship between the CCM approach to quantum many-body theory and the so-called three-Hilbert-space formulation of quantum theory was both formal and physical. We noticed that in both of these approaches one tries to combine the idea of the availability of a straightforward, formally friendly, approximation (or of a sequence of approximations) of ψ by a simpler ψ_0, with the practical awareness of the weak points (i.e., typically, of a slowness of convergence) of the respective approach. For a formal remedy to the latter weakness one may then immediately turn to the, by now, rather standard mathematical technique of the so-called preconditioning [72–75], the essence of which lies in the use of the factorized Ansatz of Eq. (2).

5.1 Physics of time-dependent correlations

For both the CCM and three-Hilbert-space formalisms, successful examples of the practical implementation of the Hilbert-space-mapping approach abound. In just the specific context of many-fermion quantum physics, for example, we may recall, e.g., the pioneering works of Dyson [33,34], Maleev [39], Coester et al. [16,17], Čížek et al. [18,19,76], and Janssen et al. [37], in all of which the above broad approach was adopted. The subjects and applications of these papers covered a broad spectrum of applied quantum theory, including condensed-matter physics [34,77], nuclear physics [7–9,78], and the descriptions of large atoms and molecules in quantum chemistry [79,80].

The essence of all of these techniques of making predictions concerning complicated multi-particle structures may be said to lie in a combination of a systematic mathematics behind approximations (reflecting, typically, the calculation feasibility aspects) with an intuitive insight into the relevance of various competing phenomena (i.e., typically, of the various types of the correlations). Thus, in a way which motivated our present paper, a transfer of the years-long experience from the static to non-stationary systems and calculations may be perceived as a true challenge.

We came to the conclusion that a key component of such a transfer should be seen in a clear abstract formulation of the formalism itself. In this sense, we tried to propose and promote a combination of the NHIP language (emphasizing, in essence, the clear separation of the state- and operator-evolution equations) with the CCM-related constructive efficiency. We believe that such a combination will pave the way towards an increase of efficiency of the calculations, based on the use of creation and annihilation operators which is, simultaneously, linear (i.e., related to the construction of the bases) and non-linear (entering the mimicking of correlations via the judicious forms of the exponential mappings Ω).

As we have already noted, at various levels of approximate implementation of any version of the CCM a loss of manifest Hermiticity between corresponding ket and bra states can arise from one of its basic tenets, viz. that formally the ground ket and bra states are parametrized independently [2,5]. In practice any potential shortcomings that this may give rise to are far outweighed by the fact that in so doing one ensures the exact maintenance of the important Hellmann–Feynman theorem [20,21] at all such levels of approximation (and see Ref. [10] for details). Thus, calculations of the ground-state expectation values of a Hermitian operator $\mathfrak{q}$ that represents an arbitrary observable quantity are completely compatible with those for the energy expectation value, in the sense that the former can be obtained from the usual (perturbation-theoretical) Goldstone diagrams for the energy by replacing in turn each interaction term in $\mathfrak{h}$ by the operator $\mathfrak{q}$.

5.2 The role and interpretation of the creation and annihilation operators

One of the strongest motivations of our present goals of uncovering a reinterpretation and translation of the TD-CCM techniques into the NHIP language (and *vice versa*) may be sought in the key merits of the CCM recipe in which one relies, heavily, upon the traditional explicit use of creation and annihilation operators, as discussed in detail in Sect. 2. This is a decisive merit which reflects our experience, intuition and pragmatic perception of the underlying phenomenology, especially when one deals with correlations carrying certain characteristic features of the quantum particle clustering. Moreover, the explicit use of the concept of clusters also leads to multiple vital simplifications of the explicit constructive calculations.

In the opposite direction, in the NHIP language one shifts attention to several related abstract concepts, such as the correspondence principle and some of its less obvious consequences [14,81]. The conservation of probabilities, which is guaranteed by the underlying unitarity of the temporal evolution in our non-Hermitian pictures is thence put in a new perspective, especially because in the non-stationary dynamical regime the energy clearly then ceases to be conserved. The related operator will represent just the instantaneous total energy.

The NHIP framework seems more (perhaps, even too) general and abstract in most application-oriented contexts. At the same time we saw previously [1], that the very essential advantage gained by building bridges between the NHIP-related and CCM-related constructions could be viewed as a certain optimal balance between the abstract concepts making use of an explicit reference to the specific features of the systems and operators in question.

The respective implementations of the Ansatz of Eq. (2) were largely inspired by the traditional Hartree–Fock methods, which were themselves based on the choice of an (often interaction-independent) Slater determinant ψ_0. These approximations were then systematically upgraded to, e.g., the most sophisticated non-Hermitian versions of the CCM as described and applied to a wide variety of physical systems in, e.g., Refs. [2–6,10,16–19,23,28,76–80,82–107]. For a broad and general overview of the CCM and its applications we may recommend the interested reader to the specific reviews contained in Refs. [6,10,80,108].

We discussed in Sect. 2 how the NCCM and ECCM parametrizations of an arbitrary quantum many-body theory enable it to be mapped *exactly* onto a classical Hamiltonian mechanics for the many-body, classical (*c*-number) configuration-space amplitudes that completely and exactly describe the ket and bra ground states independently. As we saw explicitly, these mappings arise fundamentally from an underlying one-to-one correspondence that can be proven to exist between the set of commutators in the original quantum many-body Hilbert space and a set of suitably defined generalized classical Poisson brackets.

It has further been shown [3] how the CCM (particularly in its ECCM form) can be interpreted as an *exact* generalized mean-field theory (i.e. beyond the Hartree–Fock level) formulation of the given quantum many-body problem. This interpretation is itself closely linked with the additional realization that the ECCM can also be construed as an *exact* bosonization procedure in which the ECCM states are associated in a one-to-one fashion with a set of generalized coherent states in some suitably defined boson space. This ECCM bosonization procedure differs from other such procedures in the sense that the usual motivation for any bosonization scheme is taken to its logical conclusion, viz. that the resultant generalized coherent boson fields are classical *c*-number fields with only classical (but highly nonlinear) interactions between them. Being able to reinterpret the ECCM as an exact generalized mean-field theory is then reinforced by being able to show that, within the ECCM

bosonization scheme, commutators of operators in the original Hilbert space are mapped only onto the *tree-level* pieces of the corresponding commutators of the respective mapped operators in their boson image space. The tree level of a commutator is here defined to be a restriction only to such contractions that do not result in closed loops. The subsequent manifest exclusion of all closed-loop diagrams thus acts to further reinforce the fact that the ECCM exactly reformulates the quantum-mechanical many-body system that we start with as a classical generalized mean-field theory.

6 Illustrative examples of the TD-CCM approaches

6.1 The Rabi model revisited

In view of our general discussions in Sects. 2 and 4 of the fundamentals of the TD-CCM and NHIP formalisms, respectively, and the overlaps that we have seen exist between them, we can now appreciate how the use of the multi-configurational creation operators $\{C_I^+\}$ and their destruction counterparts $\{C_I^-\}$ in the NCCM parametrizations of Eqs. (11) and (12) leads to a technically feasible implementation of the NHIP concepts, via the associated use of the c-number cluster correlation coefficients defined in Eq. (12), as we now again illustrate.

Thus, firstly, in Sect. 2.3 we outlined the basic ideas behind a prototypical application of the stationary version of the NCCM to the specific case of the Rabi model, whose Hamiltonian is as specified in Eq. (50). The model has also been studied in the non-stationary regime using the time-dependent version of the NCCM [29], in which the basic coefficients $\{s_n^{(i)}, \tilde{s}_n^{(i)}; i = 1, 2\}$ of Eqs. (54a) and (54b) now become time-dependent, and the problem reduces in practice to solving their evolution equations (22) in the same SUB-N approximation hierarchy discussed in Sect. 2.3.

Perhaps the most important atomic quantity of interest associated with the Rabi model, particularly since it is amenable to experimental observation [109], is the so-called *atomic inversion*, viz. $\langle \sigma^z \rangle(t)$. It is easy to show that in the NCCM parametrization of Sect. 2.3 it may be calculated as follows,

$$\langle \sigma^z \rangle(t) = -1 + 2 \sum_{n=1}^{\infty} \tilde{s}_n^{(2)}(t)\, s_n^{(2)}(t) .$$

(78)

Similarly, the most important field observable is the photon number, whose associated operator is $\mathfrak{n} = b^\dagger b$. Once again, it is easily shown that its time-dependent expectation value has the simple NCCM parametrization,

$$\langle \mathfrak{n} \rangle(t) = \sum_{n=1}^{\infty} n\tilde{s}_n^{(1)}(t)\, s_n^{(1)}(t) + \sum_{n=2}^{\infty} (n-1)\tilde{s}_n^{(2)}(t)\, s_n^{(2)}(t) .$$

(79)

As was done in Ref. [29], an obvious choice of initial condition at time $t = t_0$ to illustrate the efficacy of the method is to start the system in the reference state itself, i.e., the state $|0\rangle|\downarrow\rangle$, which comprises an empty field mode and an unexcited atom, for which $s_n^{(i)}(t_0) = 0 = \tilde{s}_n^{(i)}(t_0)$ for $i = 1, 2$.

As observables, both $\langle \sigma^z \rangle(t)$ and $\langle \mathfrak{n} \rangle(t)$ should always be real. However, the SUB-N truncations of the NCCM cluster operators inevitably leads to the exact Hermiticity of the corresponding bra and ket states being broken, which means that observables are not constrained to be manifestly real at any such level of approximation. Calculations show (and

see Ref. [29]) that for small values of the coupling g the imaginary parts of the observables are extremely small, and decrease as the truncation index N is increased. Thus, for relatively small couplings the evolutions of the calculated values of $\langle \sigma^z \rangle(t)$ and $\langle \mathfrak{n} \rangle(t)$ clearly show [29] a (quasi-)periodic exchange of energy between the atom and the field. Nevertheless, as g is increased, the restriction on the maximum SUB-N level that can be attained in practice for higher couplings, ensures that any spurious complex parts cannot be entirely eliminated. Thus, although the source of the errors is well known, a mathematically robust and well-founded means to suppress, and eventually eliminate, them remains unknown. One of our hopes now is that a resolution of the error-control puzzle might be provided by establishing a deeper correspondence between the NHIP-related abstract "bookkeeping" of the relevant operator evolution equations, and the various pragmatic CCM solution techniques. A best possible outcome would thereby be to improve upon the standard CCM SUB-N truncation hierarchy. We return to this point below after discussing our second illustrative example of an application of the TD-CCM formalism.

Before doing so, however, we remind the reader that the above simple choice of initial conditions was made purely for ease. Other choices are certainly possible, and for an arbitrary physical state as the starting state, we can always first calculate its NCCM representation to yield its corresponding coefficients $\{s_n^{(i)}, \tilde{s}_n^{(i)}; i = 1, 2\}$, which may then be taken as the initial conditions at $t = t_0$.

6.2 Condensed Bose fluid

We now turn to our second, much more ambitious, example of an application of the TD-CCM, viz. to describe the zero-temperature hydrodynamics of a macroscopic condensed Bose fluid, this time via the ECCM [110]. A convenient choice of reference state for this model is now $|\psi_0\rangle = |0\rangle$, the bare vacuum. Accordingly, we are thus working in a number-nonconserving formulation, as introduced by Bogolubov [111]. Particle-number conservation is then imposed by working with the grand canonical Hamiltonian $\mathfrak{k}_{(0)} \equiv \mathfrak{h}_{(0)} - \mu \mathfrak{n}$ rather than with the Hamiltonian, $\mathfrak{h}_{(0)}$, where μ is the chemical potential and $\mathfrak{n}$ is the particle number operator. We consider here a system of N identical bosons, each of mass m and interacting via pairwise potentials, such that (in first quantization),

$$\mathfrak{h}_{(0)} = -\frac{1}{2m} \sum_{j=1}^{N} \nabla_j^2 + \sum_{i=1}^{N} \sum_{j<i} \mathfrak{v}(\mathbf{x}_i - \mathbf{x}_j) . \tag{80}$$

We parametrize the many-body configuration space in terms of real-space coordinates, such that the single-boson creation and destruction operators, $b^\dagger(\mathbf{x})$ and $b(\mathbf{x})$, respectively, which act to create or annihilate a particle at the three-space point $\mathbf{x} \equiv (x_1, x_2, x_3)$, obey the usual bosonic commutation relations, $[b(\mathbf{x}), b^\dagger(\mathbf{y})] = \delta^{(3)}(\mathbf{x} - \mathbf{y})\mathbb{1}$. In the original Hilbert space with fixed particle number N, Eq. (10) now takes the specific form,

$$\mathbb{1} = \sum_{n=0}^{\infty} \frac{1}{n!} \int d\mathbf{x}_1 \cdots \int d\mathbf{x}_n \, b^\dagger(\mathbf{x}_1) \cdots b^\dagger(\mathbf{x}_n)|0\rangle\langle 0|b(\mathbf{x}_n) \cdots b(\mathbf{x}_1) . \tag{81}$$

Correspondingly, the generic ECCM amplitudes of Eqs. (38) and (41) now also take the specific forms,

$$\Sigma(t) = \sum_{n=1}^{\infty} \frac{1}{\sqrt{n!}} \int d\mathbf{x}_1 \cdots \int d\mathbf{x}_n \, \sigma_n(\mathbf{x}_1, \cdots, \mathbf{x}_n; t) \, b^\dagger(\mathbf{x}_1) \cdots b^\dagger(\mathbf{x}_n) , \tag{82a}$$

$$\tilde{\Sigma}(t) = \sum_{n=1}^{\infty} \frac{1}{\sqrt{n!}} \int d\mathbf{x}_1 \cdots \int d\mathbf{x}_n \, \tilde{\sigma}_n(\mathbf{x}_1, \cdots, \mathbf{x}_n; t) \, b(\mathbf{x}_n) \cdots b(\mathbf{x}_1) . \tag{82b}$$

We can now see immediately that the ECCM formalism of Sect. 2.2 provides a framework in which to consider the general case of a non-stationary and spatially non-uniform condensate, $\langle b(\mathbf{x}) \rangle(t) = \langle \psi_0 | e^{\tilde{\Sigma}(t)} e^{-S(t)} b(\mathbf{x}) e^{S(t)} | \psi_0 \rangle$. Indeed, by making use of Eqs. (14b) and (15) and the fact that $S(t)$ has a corresponding expansion to that for $\Sigma(t)$ in Eq. (82a), we see that $e^{-S(t)} b(\mathbf{x}) e^{S(t)} = b(\mathbf{x}) + [b(\mathbf{x}), S(t)]$. Finally, use of the relation $b(\mathbf{x})|\psi_0\rangle = 0$ then shows that

$$\langle b(\mathbf{x}) \rangle(t) = \langle \psi_0 | e^{\tilde{\Sigma}(t)} b(\mathbf{x}) S(t) | \psi_0 \rangle = \langle \psi_0 | b(\mathbf{x}) e^{\tilde{\Sigma}(t)} S(t) | \psi_0 \rangle = \sigma_1(\mathbf{x}; t) , \tag{83}$$

where the last equality follows from the generic definition of Eq. (42). Thus the condensate wave function $\langle b(\mathbf{x}) \rangle(t)$ is precisely given by the one-body ECCM amplitude $\sigma_1(\mathbf{x}; t)$. Thus, it is no surprise to learn that at the lowest SUB-1 (i.e., one-body mean-field) level of truncation of the general SUB-N hierarchy (in which all ECCM amplitudes σ_n and $\tilde{\sigma}_n$ with $n > N$ are set to zero) our formalism simply reduces to the well-known Gross–Pitaevskii [112,113] description of the condensate wave function (or one-body order parameter). Hence, our usual SUB-N approximation hierarchy can now be used to improve systematically upon this lowest-order one-body mean-field description.

In order to take full advantage of the local $U(1)$ gauge symmetry that follows from particle-number conservation it is now very convenient to couple the system to external $U(1)$ *gauge fields* $\phi(\mathbf{x}, t)$ and $\mathbf{A}(\mathbf{x}, t)$ (viz. the scalar and vector potentials, respectively), and hence we now study the new grand canonical Hamiltonian $\mathfrak{k}$, where (in first quantization),

$$\mathfrak{k} \equiv \sum_{j=1}^{N} \frac{1}{2m} \big[-i\nabla_j - \mathbf{A}(\mathbf{x}_j, t) \big]^2 + \sum_{j=1}^{N} \big[\phi(\mathbf{x}_j, t) - \mu \big] + \sum_{i=1}^{N} \sum_{j<i} \mathfrak{v}(\mathbf{x}_i - \mathbf{x}_j) . \tag{84a}$$

Equation (84a) may be equivalently rewritten in the second-quantized form,

$$\begin{aligned}
\mathfrak{k} = {} & \frac{1}{2m} \int d\mathbf{x} \big[\nabla_x b^\dagger(\mathbf{x}) \big] \cdot \big[\nabla_x b(\mathbf{x}) \big] \\
& + \frac{i}{2m} \int d\mathbf{x} \, \mathbf{A}(\mathbf{x}, t) \cdot \big\{ b^\dagger(\mathbf{x}) \big[\nabla_x b(\mathbf{x}) \big] - \big[\nabla_x b^\dagger(\mathbf{x}) \big] b(\mathbf{x}) \big\} \\
& + \int d\mathbf{x} \big[\phi(\mathbf{x}, t) - \mu + \frac{1}{2m} \mathbf{A}^2(\mathbf{x}, t) \big] b^\dagger(\mathbf{x}) b(\mathbf{x}) \\
& + \frac{1}{2} \int d\mathbf{x} \int d\mathbf{y} \, \mathfrak{v}(\mathbf{x} - \mathbf{y}) b^\dagger(\mathbf{x}) b^\dagger(\mathbf{y}) b(\mathbf{y}) b(\mathbf{x}) .
\end{aligned} \tag{84b}$$

Using this grand canonical Hamiltonian $\mathfrak{k}$ as the time-evolution operator, one may now explicitly evaluate [110] the equations of motion (46) (with $\mathbb{H} \to \mathbb{K}$) for the ECCM amplitudes $\{\sigma_n, \tilde{\sigma}_n\}$. The whole treatment may now be developed in a completely gauge-invariant fashion so as to provide a complete (zero-temperature) hydrodynmical description. In particular, one may study the evolution of the expectation values of the off-diagonal one- and two-body density operators. One can thereby derive in a wholly gauge-invariant form the exact balance equations (i.e., the local conservation laws) for the hydrodynamically relevant

variables (viz. the particle-number density, current density, and energy density, all considered as functions of spatial position and time), and show how these are in turn related to (and derivable from) the cumulant expansion of the one-body density matrix. It has also been shown [110] that each of the balance equations is exactly obeyed at every SUB-N level of truncation.

We note that the $U(1)$ gauge invariance that we have been at pains to incorporate exactly, can, of course, itself be interpreted as the (differential or) local Galilean invariance. An immediate consequence is that the description correctly separates the average translational (hydrodynamical) kinetic energy from the average kinetic energy in the local rest frame, which has otherwise proven to be very difficult to achieve in a fully microscopic treatment. One can clearly reinterpret this exact feature of the time-dependent ECCM treatment of a condensed Bose fluid with the generic proper treatment within the NHIP of the analogous Coriolis terms $\Xi(t)$ of Eq. (72) in the evolution generator operator $G(t)$. Despite being beyond the scope of the present paper, it would be interesting in this light to pursue this relationship further, since one might expect it to extend our intuitive insight into both methods, as well as to lead possibly to improved computational (i.e., approximation) schemes.

Before closing this discussion, however, we note that the temporal evolution of the system has been described by a trajectory in the ECCM symplectic phase space spanned by the cluster coefficients $\{\sigma_n, \tilde{\sigma}_n\}$. The modern viewpoint of statistical mechanics [22], however, is that a proper qualitative description of the system is obtained, rather, from the entire *phase portrait*, which is just the totality of all allowed trajectories. From this stance, it is clear that the above single-trajectory ECCM approach might now usefully be extended by focusing more on the geometric properties of the ECCM phase space, as have been discussed in some detail in Ref. [96]. By contrast, we have so far focused more on the algebraic structure of the ECCM phase space (and see Ref. [95] for further details), and in so doing we have been led inexorably to the SUB-N hierarchy of approximations. As we have seen in Sect. 2.3, for example, this scheme sometimes has computational limitations, which stem essentially from the fact that, although the ECCM has left its ultimate origins in perturbation theory far behind, the SUB-N scheme itself does still seem to have some links with perturbation theory. The hope has been expressed [110] that one might be able to exploit the geometric structure of the ECCM phase space to derive wholly new (and potentially more robust and more powerful) approximation schemes based wholly on its geometric properties. Again, we note that, although such an investigation lies beyond the scope of the present paper, any progress in this area will certainly find immediate impact in the NHIP formalism too.

7 Outlook

In the arena of realistic and predictive CCM calculations, most attention is usually paid to the study of molecules and/or other quantum many-body systems in their ground state. Once our interest shifts to the excited states the strategy has to be modified, as we alluded to in Sect. 3. Within the S-CCM such a modification was first proposed by Emrich [83,84] within the context of the time-independent (i.e., stationary) Schrödinger equation. This was done by a suitable modification of the ground-state parametrization, which did not involve a change of reference state. A later alternative TD-CCM approach to excited states was advocated by Arponen and his co-workers [2,4] within the context of the time-dependent Schrödinger equation, wherein it was shown how excited states could be obtained as the normal modes of a suitably defined dynamical Hamiltonian matrix obtained within linear response theory, in direct analogy to the usual procedure in classical mechanics. The complete equivalence of

the two approaches has been formally demonstrated [4,5,10]. In effect, what we have done in the present paper is to build upon, and extend, these results.

7.1 Reference-dependence versus reference-independence

In the broader context of constructive quantum many-body theory the key purpose of our present paper may be seen in the description of the close relationship between the reference-dependent and reference-independent forms of the Ansatz of Eq. (2). In this sense our present study of parallels between the alternative NHIP and TD-CCM approaches to non-stationary dynamics was preceded by our earlier paper [1] in which the methodical framework was perceivably simplified and reduced to the less sophisticated search for parallels between the stationary DMF and S-CCM methods.

As a concise summary of the message provided by Ref. [1] it can be said that the reconsideration of the S-CCM method from the reference-independent DMF perspective may be well illustrated in diagrammatic form by the flowchart in our present Eq. (56). Therein one assumes an input knowledge of the Hamiltonian operator $\mathfrak{h}$ and of the Dyson mapping Ω. In this setting the main weakness of the reference-independent DMF recipe lies in the absence of any hint of how we should choose the operator map Ω. Hence, the stationary DMF approach may, somewhat crudely, but simply, be characterized as guesswork, or as an intuition-based implementation of a purely trial-and-error-type strategy.

This does not mean that the DMF constructions were not successful in practice. In fact, the opposite is true [32]. Still, the S-CCM techniques are more systematic because, given a Hamiltonian operator $\mathfrak{h}$, the S-CCM specification of the necessary Dyson operator $\Omega = \exp S$ is not at all arbitrary, with the rationale for the exponentiated form as we have outlined above. Hence, the S-CCM techniques are both "algorithmic" and extremely intuitive. A related major advantage of the S-CCM lies in the use of the very concrete truncated-series expansions of the Dysonian exponent operator S in an operator basis formed by certain multi-configurational creation operators, as alluded to above. This opens the dual possibilities of multiple technical simplifications and extremely powerful approximation hierarchies that are well-defined and physically motivated, both of which are *precisely due to* the intrinsic reference-dependence of the S-CCM construction.

In the present paper we have pointed out that a similar balance between the merits and shortcomings must also necessarily exist (and should prove useful) when one replaces the S-CCM $\leftrightarrow$ DMF stationary correspondence by its TD-CCM $\leftrightarrow$ NHIP time-dependent generalization. *A priori* one may expect that in the generalized setting, *any* technical simplification (obtained from the mutual enrichment) could play a more decisive role, first of all, because of the enormous overall increase in mathematical complexity that emerges after the respective replacements S-CCM $\rightarrow$ TD-CCM and/or DMF $\rightarrow$ NHIP.

Particular attention has to be paid to a deeper theoretical role played by the transfer of mathematical know-how from the DMF and NHIP formalisms to their respective S-CCM and TD-CCM counterparts. In this manner the brute-force S-CCM and TD-CCM constructions appear open to further amendments. A typical example is the possible replacement of a certain *ad hoc*, auxiliary S-CCM or TD-CCM operator admitted by the principles of bivariationality, and hence needed to characterize the bra states *independently* from the ket states (viz. the operator $\tilde{S}$ in the NCCM or $\tilde{\Sigma}$ in the ECCM) that is thus required for the evaluation of the expectation values of an arbitrary physically observable operator, by alternative forms that maintain the canonical CCM symplectic structure discussed in Sect. 2, which are both inspired and restricted by the implicit mathematical merits (e.g., the Hermiticity reinstallation property) of its metric-operator-provided reinterpretation.

7.2 Interaction-picture context

Let us recall the well-known method of Seidewitz [114] for avoiding the no-go consequences of Haag's theorem in quantum field theory (QFT), which states that, under the *usual* assumptions made in QFT, any field that is unitarily equivalent to a free field must itself be a free field. In particular, Seidewitz shows how Haag's theorem can be avoided when QFT is formulated using an additional invariant *path* parameter, as well as the usual four-position parameters. His method relies on the removal of the spectral condition, essentially by replacing the usual on-mass-shell operator of relativistic energy and momentum by its off-shell generalization $\hat{P}$. Importantly, this is accompanied by the preservation of the traditional IP approach to the Dyson perturbation expansions of scattering matrices, thereby providing a fully consistent basis for performing the usual practical QFT calculations.

For the purposes of our present discussion, what is important in the above Seidewitz construction [114] is that, in order to bypass the limitations imposed by Haag's theorem in the standard formulations of QFT, the frame-dependent zeroth component of $\hat{P}$, which plays the role of the energy operator in conventional QFT, necessarily becomes different from the newly introduced free relativistic Hamiltonian. From a rather abstract point of view the latter idea is reminiscent of and, indeed, completely paralleled by, our present introduction of the distinctions between several alternative candidates to play the role of a non-stationary non-Hermitian Hamiltonian.

As we have seen, only one of these candidates (viz. the IP operator $H(t)$) is hiddenly Hermitian (i.e., observable). The other ones [viz. the IP operators $\mathcal{E}(t)$ and $G(t)$], together with their conjugate forms are not. In general, the differences $[G^{\dagger}(t) - G(t)]$ and $[\mathcal{E}^{\dagger}(t) - \mathcal{E}(t)]$ do not vanish. In turn, this opens up a wide space for multiple unconventional dynamical scenarios that provide an interplay and mutual cancellations between the non-unitarily evolving components in states $\psi(t)$ and in observables $Q(t)$, respectively. Along these lines, the ultimate (hidden) unitarity of the whole picture is achieved.

We described the corresponding non-Hermitian generalizations of evolution equations, thereby offering a firm ground for the transfer (NHIP → TD-CCM) of the *operator* NHIP formalism into its *variational* TD-CCM parallels. In the present stage of development of the theory we already understand why and how operators $G(t)$ and $G^{\dagger}(t)$ control the time-evolution of states, as well as why and when their Coriolis-operator partners $\mathcal{E}(t)$ and $\mathcal{E}^{\dagger}(t)$ play the role of the generators of time-evolution of all of the IP-represented observables. As two specific examples of where the opposite transfer (TD-CCM → NHIP) of experience from the TD-CCM to its NHIP counterpart might lead to further insights we recall the specific applications of the former to the Rabi Hamiltonian and the condensed Bose fluid, as discussed in Sect. 6.

In the context of much recent research in the area that has been aimed mainly at the SP formalism, we have also clarified here the deep changes in the role of the so-called Hilbert space metric in the generic situations in which it is allowed to vary with time, $\Theta = \Theta(t)$. Furthermore, having shown here how we can, completely equivalently, work instead solely with the *pairs* $\{|\psi(t)\rangle, |\psi(t)\rangle\rangle\}$ of the single-state-representing kets and ketkets, we also thereby demonstrated how the explicit need for the operator $\Theta(t)$ itself has certainly been weakened, if not altogether eliminated. We believe that a transfer of this experience to the variational context is potentially extremely productive.

8 Summary

The formulation of the relationships illustrated in Eq. (59) was motivated, first of all, by the many phenomenological successes of the conventional stationary special case of Eq. (56). In the present paper, the emphasis was aimed rather at an innovative reinterpretation of the existing non-stationary (TD-CCM) extensions of the variational CCM techniques.

The underlying mathematical and technical details required to transfer the non-stationary Dyson-inspired formalism (viz. the NHIP approach) were outlined. It is precisely in this domain where a large part of our present contributions are truly original in their own right. The remaining originality resides in bringing into juxtaposition, within a newly developed conceptual and notational framework that is broad and powerful enough to encompass both, two very powerful methodologies that have hitherto been seen as quite separate. We have been at some pains to draw parallels that might henceforth be exploited to advance both formalisms and their subsequently enhanced arenas of applications. We have described in some detail how the key source of the mathematical inspiration for our study lies in the unconventional *non-Hermiticity* of Hamiltonians in the formalisms. This gave birth earlier [1] to the explicit, and rather fruitful, description of manifold conceptual parallels between two otherwise seemingly disparate theoretical constructs. These comprise, on one hand, the very successful stationary S-CCM formulations of quantum many-body theory and, on the other, their (at least, in principle) somewhat more ambitious, quasi-Hermitian [32–34,70] (otherwise known as pseudo-Hermitian [14] or $\mathcal{PT}$-symmetric [13]) *stationary* analogues, which, by now, have themselves also become rather widely used in a variety of applications of quantum theory.

A non-stationary, TD-CCM version of the CCM theory has been considered here, therefore. This was done because we believe that, in contrast to the rather universal Dyson-inspired quasi-Hermiticity techniques, a characteristic and specific merit of the less universal CCM theory may be seen in the much larger number of very accurate calculations that it has found in such a wide range of applications in many diverse subfields of quantum physics and chemistry.

Several conclusions from our study also appear to provide a perceptibly deeper insight into abstract quantum theory itself. In particular, we have shown that one can easily remove the representation-framework restrictions as accepted both in Ref. [11] (wherein only wave functions evolved in time, i.e., in the non-Hermitian Schrödinger picture) and in Ref. [46] (where the transition to the non-Hermitian Heisenberg picture, in which wave functions remain constant in time, was analyzed). In other words, our present version of the NHIP formalism (in which both wave functions and operators of observables cease to remain constant in time) may be briefly characterized as an immediate non-Hermitian generalization of the interaction picture (alias the traditional Dirac picture) as described in most standard quantum mechanics textbooks (and see, e.g., Refs. [115–117]), and as now almost universally used in quantum field theory calculations (and see, e.g., Refs. [58,59,118–120]).

One of the deep unifying features between the quasi-Hermiticity techniques on the one hand and the CCM on the other is their ability to be formulated in terms of a bivariational principle. For the general case of quasi-Hermitian operators in quantum mechanics, Scholtz et al. [32] showed in particular how the introduction of the metric operator was especially useful for the implementation of a variational principle, which could itself then be used for (approximate) calculational purposes. Exactly the same bivariational formulation of both S-CCM and TD-CCM approaches [2,5] has led to the extremely accurate descriptions of a wide variety of strongly-interacting quantum many-body systems.

Another common feature of the quasi-Hermiticity and CCM (particularly the ECCM) formalisms is their deep relationship to exact bosonization mappings. In the case of the ECCM this has even resulted in its ultimate realization as an exact *classicization* [3], as we discussed in some detail in Sect. 5.2. The ECCM itself, as we also discussed, introduces *two* independent preconditioning operators Ω of the form of Eq. (4). We now fully expect that this important feature of the ECCM might also find applications into a further useful, parallel extension of the three-Hilbert-space (alias the NHIP) formalism, which mirrors the NCCM $\rightarrow$ ECCM extension. However, such a discussion takes us far beyond the aims of the present paper.

References

1. R.F. Bishop, M. Znojil, Acta Polytech. **54**, 85 (2014). https://doi.org/10.14311/AP.2014.54.0085
2. J. Arponen, Ann. Phys. (NY) **151**, 311 (1983). https://doi.org/10.1016/0003-4916(83)90284-1
3. J.S. Arponen, R.F. Bishop, E. Pajanne, Phys. Rev. A **36**, 2519 (1987). https://doi.org/10.1103/PhysRevA.36.2519
4. J.S. Arponen, R.F. Bishop, E. Pajanne, Phys. Rev. A **36**, 2539 (1987). https://doi.org/10.1103/PhysRevA.36.2539
5. R.F. Bishop, J. Arponen, E. Pajanne, in *Aspects of Many-Body Effects in Molecules and Extended Systems*, vol. 50, Lecture Notes in Chemistry, ed. by D. Mukherjee (Springer, Berlin, 1989), pp. 79–100. https://doi.org/10.1007/978-3-642-61330-2_4
6. R.F. Bishop, Theor. Chim. Acta **80**, 95 (1991). https://doi.org/10.1007/BF01119617
7. A. Arima, F. Iachello, Ann. Phys. (NY) **99**, 253 (1976). https://doi.org/10.1016/0003-4916(76)90097-X
8. A. Arima, F. Iachello, Ann. Phys. (NY) **111**, 201 (1978). https://doi.org/10.1016/0003-4916(78)90228-2
9. A. Arima, F. Iachello, Ann. Phys. (NY) **123**, 468 (1979). https://doi.org/10.1016/0003-4916(79)90347-6
10. R.F. Bishop, in *Microscopic Quantum Many-Body Theories and Their Applications*, vol. 510, Lecture Notes in Physics, ed. by J. Navarro, A. Polls (Springer, Berlin, 1998), pp. 1–70. https://doi.org/10.1007/BFb0104523
11. M. Znojil, SIGMA **5**, 001 (2009). https://doi.org/10.3842/SIGMA.2009.001
12. F. Bagarello, J.P. Gazeau, F.H. Szafraniec, M. Znojil (eds.), *Non-Selfadjoint Operators in Quantum Physics: Mathematical Aspects* (Wiley, Hoboken, 2015). https://doi.org/10.1002/9781118855300
13. C.M. Bender, Rep. Prog. Phys. **70**, 947 (2007). https://doi.org/10.1088/0034-4885/70/6/R03
14. A. Mostafazadeh, Int. J. Geom. Methods Mod. Phys. **07**, 1191 (2010). https://doi.org/10.1142/S0219887810004816
15. J. Goldstone, Proc. R. Soc. Lond. Ser. A **239**, 267 (1957). https://doi.org/10.1098/rspa.1957.0037
16. F. Coester, Nucl. Phys. **7**, 421 (1958). https://doi.org/10.1016/0029-5582(58)90280-3
17. F. Coester, H. Kümmel, Nucl. Phys. **17**, 477 (1960). https://doi.org/10.1016/0029-5582(60)90140-1
18. J. Čížek, J. Chem. Phys. **45**, 4256 (1966). https://doi.org/10.1063/1.1727484
19. J. Čížek, in *Advances in Chemical Physics: Correlation Effects in Atoms and Molecules*, vol. 14, ed. by R. LeFebvre, C. Moser (Wiley, Hoboken, 1969), pp. 38–89. https://doi.org/10.1002/9780470143599.ch2
20. H. Hellmann, Acta Physicochim. URSS **1**, 913 (1934/1935)
21. R.P. Feynman, Phys. Rev. **56**, 340 (1939). https://doi.org/10.1103/PhysRev.56.340

22. R. Abraham, J.E. Marsden, *Foundations of Mechanics*, 2nd edn. (AMS Chelsea Publications, Providence, RI, 1978). https://doi.org/10.1090/chel/364
23. J. Arponen, Phys. Rev. A **55**, 2686 (1997). https://doi.org/10.1103/PhysRevA.55.2686
24. M. Henneaux, C. Teitelboim, *Quantization of Gauge Systems* (Princeton University Press, Princeton, 1992). https://press.princeton.edu/books/paperback/9780691037691/quantization-of-gauge-systems
25. L. Allen, J.H. Eberly, *Optical Resonance and Two-Level Atoms* (Wiley-Interscience, New York, 1975). https://doi.org/10.1002/piuz.19760070115
26. I.I. Rabi, Phys. Rev. **51**, 652 (1937). https://doi.org/10.1103/PhysRev.51.652
27. J.T. Marshall, J.L. Pell, Phys. Rev. D **24**, 394 (1981). https://doi.org/10.1103/PhysRevD.24.394
28. R.F. Bishop, N. Davidson, R.M. Quick, D.M. van der Walt, Phys. Rev. A **54**, R4657 (1996). https://doi.org/10.1103/PhysRevA.54.R4657
29. R.F. Bishop, C. Emary, J. Phys. A: Math. Gen. **34**, 5635 (2001). https://doi.org/10.1088/0305-4470/34/28/302
30. C. Emary, R.F. Bishop, J. Math. Phys. **43**, 3916 (2002). https://doi.org/10.1063/1.1490406
31. T. Holstein, H. Primakoff, Phys. Rev. **58**, 1098 (1940). https://doi.org/10.1103/PhysRev.58.1098
32. F.G. Scholtz, H.B. Geyer, F.J.W. Hahne, Ann. Phys. **213**, 74 (1992). https://doi.org/10.1016/0003-4916(92)90284-S
33. F.J. Dyson, Phys. Rev. **102**, 1217 (1956). https://doi.org/10.1103/PhysRev.102.1217
34. F.J. Dyson, Phys. Rev. **102**, 1230 (1956). https://doi.org/10.1103/PhysRev.102.1230
35. E. Schrödinger, Ann. Phys. (Berlin) **384**, 361 (1926). https://doi.org/10.1002/andp.19263840404
36. C.M. Bender, S. Boettcher, Phys. Rev. Lett. **80**, 5243 (1998). https://doi.org/10.1103/PhysRevLett.80.5243
37. D. Janssen, F. Dönau, S. Frauendorf, R.V. Jolos, Nucl. Phys. A **172**, 145 (1971). https://doi.org/10.1016/0375-9474(71)90122-9
38. M. Znojil, in *Non-Selfadjoint Operators in Quantum Physics: Mathematical Aspects*, ed. by F. Bagarello, J.P. Gazeau, F.H. Szafraniec, M. Znojil (Wiley, Hoboken, NJ, USA, 2015), pp. 7–58. https://doi.org/10.1002/9781118855300.ch1
39. S.V. Maleev, Zh. Eksp. Teor. Fiz. **33**, 1010 (1957). http://www.jetp.ac.ru/cgi-bin/e/index/r/33/4/p1010?a=list. [translated into English in Sov. Phys. JETP **6**, 776–784 (1958)]
40. S.T. Beliaev, V.G. Zelevinsky, Nucl. Phys. **39**, 582 (1962). https://doi.org/10.1016/0029-5582(62)90416-9
41. J. Schwinger, US AEC Report **NYO-3071**, 1 (1952). https://doi.org/10.2172/4389568. [republished in *Quantum Theory of Angular Momentum*, edited by L. C. Biedenharn and H. van Dam (Academic Press, New York, 1965) p. 229]
42. T. Marumori, M. Yamamura, A. Tokunaga, Prog. Theor. Phys. **31**, 1009 (1964). https://doi.org/10.1143/PTP.31.1009
43. B. Sørensen, Nucl. Phys. A **97**, 1 (1967). https://doi.org/10.1016/0375-9474(67)90767-1
44. M. Znojil, Phys. Rev. D **78**, 085003 (2008). https://doi.org/10.1103/PhysRevD.78.085003
45. M. Znojil, Int. J. Theor. Phys. **52**, 2038 (2013). https://doi.org/10.1007/s10773-012-1451-9
46. M. Znojil, Phys. Lett. A **379**, 2013 (2015). https://doi.org/10.1016/j.physleta.2015.06.042
47. M. Znojil, Ann. Phys. (NY) **385**, 162 (2017). https://doi.org/10.1016/j.aop.2017.08.009
48. C.F. de Morisson Faria, A. Fring, J. Phys. A: Math. Gen. **39**, 9269 (2006). https://doi.org/10.1088/0305-4470/39/29/018
49. C.F.M. Faria, A. Fring, Laser Phys. **17**, 424 (2007). https://doi.org/10.1134/S1054660X07040196
50. H. Bíla, Non-Hermitian operators in quantum physics. Ph.D. thesis, Charles University, Prague, Czech Republic (2008)
51. H. Bíla, Adiabatic time-dependent metrics in PT-symmetric quantum theories. eprint arXiv:0902.0474 (2009)
52. J. Gong, Q.H. Wang, Phys. Rev. A **82**, 012103 (2010). https://doi.org/10.1103/PhysRevA.82.012103
53. J. Gong, Q.H. Wang, J. Phys. A: Math. Theor. **46**, 485302 (2013). https://doi.org/10.1088/1751-8113/46/48/485302
54. M. Maamache, Phys. Rev. A **92**, 032106 (2015). https://doi.org/10.1103/PhysRevA.92.032106
55. F.S. Luiz, M.A. de Ponte, M.H.Y. Moussa, Unitarity of the time-evolution and observability of non-Hermitian Hamiltonians for time-dependent Dyson maps. eprint arXiv:1611.08286 (2016)
56. B. Khantoul, A. Bounames, M. Maamache, Eur. Phys. J. Plus **132**, 258 (2017). https://doi.org/10.1140/epjp/i2017-11524-7
57. W. Heisenberg, Z. Phys. **33**, 879 (1925). https://doi.org/10.1007/BF01328377
58. J.D. Bjorken, S.D. Drell, *Relativistic Quantum Fields*, 1st edn. (McGraw-Hill, New York, 1965)
59. J.W. Negele, H. Orland, *Quantum Many-Particle Systems*, revised edn. (Westview Press, Boulder, CO, 1998)

60. D.F. Styer, M.S. Balkin, K.M. Becker, M.R. Burns, C.E. Dudley, S.T. Forth, J.S. Gaumer, M.A. Kramer, D.C. Oertel, L.H. Park, M.T. Rinkoski, C.T. Smith, T.D. Wotherspoon, Am. J. Phys. **70**, 288 (2002). https://doi.org/10.1119/1.1445404
61. A. Mostafazadeh, Phys. Lett. B **650**, 208 (2007). https://doi.org/10.1016/j.physletb.2007.04.064
62. M. Znojil, Time-dependent quasi-Hermitian Hamiltonians and the unitarity of quantum evolution. eprint arXiv:0710.5653 (2007)
63. A. Mostafazadeh, Comment on 'Time-dependent quasi-Hermitian Hamiltonians and the unitarity of quantum evolution'. eprint arXiv:0711.0137 (2007)
64. M. Znojil, Reply to Comment on 'Time-dependent quasi-Hermitian Hamiltonians and the unitarity of quantum evolution'. eprint arXiv:0711.0514 (2007)
65. M. Znojil, Which operator generates time evolution in quantum mechanics? eprint arXiv:0711.0535 (2007)
66. A. Mostafazadeh, Comment on 'Reply to Comment on Time-dependent quasi-Hermitian Hamiltonians and the unitarity of quantum evolution'. eprint arXiv:0711.1078 (2007)
67. A. Fring, M.H.Y. Moussa, Phys. Rev. A **93**, 042114 (2016). https://doi.org/10.1103/PhysRevA.93.042114
68. A. Fring, M.H.Y. Moussa, Phys. Rev. A **94**, 042128 (2016). https://doi.org/10.1103/PhysRevA.94.042128
69. Y.G. Miao, Z.M. Xu, Phys. Lett. A **380**, 1805 (2016). https://doi.org/10.1016/j.physleta.2016.03.035
70. J. Dieudonné, in *Proceedings of the International Symposium on Linear Spaces: held at the Hebrew University of Jerusalem, July 5-12, 1960*. The Israel Academy of Sciences and Humanities (Pergamon Press, Oxford, 1961), pp. 115–122
71. J.P. Williams, Proc. Am. Math. Soc. **20**, 121 (1969). https://doi.org/10.1090/S0002-9939-1969-0233230-5
72. M. Benzi, J. Comput. Phys. **182**, 418 (2002). https://doi.org/10.1006/jcph.2002.7176
73. K. Chen, *Matrix Preconditioning Techniques and Applications* (Cambridge University Press, 2005). http://www.cambridge.org/gb/academic/subjects/mathematics/numerical-analysis/matrix-preconditioning-techniques-and-applications?format=HB#GLZHgLFaulTPYxuR.97
74. H.A. van der Vorst, *Iterative Krylov Methods for Large Linear Systems* (Cambridge University Press, 2009). http://www.cambridge.org/gb/academic/subjects/mathematics/numerical-analysis/iterative-krylov-methods-large-linear-systems?format=PB#aDojVtAeCcRIscOe.97
75. J. Liesen, Z. Strakos, *Krylov Subspace Methods: Principles and Analysis* (Oxford University Press, 2012). https://global.oup.com/academic/product/krylov-subspace-methods-9780199655410?q=Krylov%20subspace%20methods%20:%20principles%20and%20analysis&lang=en&cc=gb#
76. J. Čížek, J. Paldus, Int. J. Quantum Chem. **5**, 359 (1971). https://doi.org/10.1002/qua.560050402
77. R.F. Bishop, P.H.Y. Li, C.E. Campbell, AIP Conf. Proc. **1619**, 40 (2014). https://doi.org/10.1063/1.4899216
78. H. Kümmel, K.H. Lührmann, J.G. Zabolitzky, Phys. Rep. **36**, 1 (1978). https://doi.org/10.1016/0370-1573(78)90081-9
79. H.J. Monkhorst, Int. J. Quantum Chem. Quantum Chem. Symp. **11**, 421 (1977). https://doi.org/10.1002/qua.560120850
80. R.J. Bartlett, M. Musiał, Rev. Mod. Phys. **79**, 291 (2007). https://doi.org/10.1103/RevModPhys.79.291
81. A. Mostafazadeh, Phys. Rev. D **98**, 046022 (2018). https://doi.org/10.1103/PhysRevD.98.046022
82. R.F. Bishop, K.H. Lührmann, Phys. Rev. B **17**, 3757 (1978). https://doi.org/10.1103/PhysRevB.17.3757
83. K. Emrich, Nucl. Phys. A **351**, 379 (1981). https://doi.org/10.1016/0375-9474(81)90179-2
84. K. Emrich, Nucl. Phys. A **351**, 397 (1981). https://doi.org/10.1016/0375-9474(81)90180-9
85. R.F. Bishop, K.H. Lührmann, Phys. Rev. B **26**, 5523 (1982). https://doi.org/10.1103/PhysRevB.26.5523
86. H. Kümmel, Phys. Rev. C **27**, 765 (1983). https://doi.org/10.1103/PhysRevC.27.765
87. C.S. Hsue, H. Kümmel, P. Ueberholz, Phys. Rev. D **32**, 1435 (1985). https://doi.org/10.1103/PhysRevD.32.1435
88. M. Altenbokum, H. Kümmel, Phys. Rev. D **32**, 2014 (1985). https://doi.org/10.1103/PhysRevD.32.2014
89. G. Hasberg, H. Kümmel, Phys. Rev. C **33**, 1367 (1986). https://doi.org/10.1103/PhysRevC.33.1367
90. U. Kaulfuss, M. Altenbokum, Phys. Rev. D **35**, 609 (1987). https://doi.org/10.1103/PhysRevD.35.609
91. M. Funke, U. Kaulfuss, H. Kümmel, Phys. Rev. D **35**, 621 (1987). https://doi.org/10.1103/PhysRevD.35.621
92. J.S. Arponen, R.F. Bishop, Ann. Phys. (NY) **207**, 171 (1991). https://doi.org/10.1016/0003-4916(91)90183-9
93. J.F. Stanton, R.J. Bartlett, J. Chem. Phys. **98**, 7029 (1993). https://doi.org/10.1063/1.464746
94. R.F. Bishop, A.S. Kendall, L.Y. Wong, Y. Xian, Phys. Rev. D **48**, 887 (1993). https://doi.org/10.1103/PhysRevD.48.887

95. J.S. Arponen, R.F. Bishop, Ann. Phys. (NY) **227**, 275 (1993). https://doi.org/10.1006/aphy.1993.1082
96. J.S. Arponen, R.F. Bishop, Ann. Phys. (NY) **227**, 334 (1993). https://doi.org/10.1006/aphy.1993.1083
97. M. Funke, H.G. Kümmel, Phys. Rev. D **50**, 991 (1994). https://doi.org/10.1103/PhysRevD.50.991
98. S.J. Baker, R.F. Bishop, N.J. Davidson, Phys. Rev. D **53**, 2610 (1996). https://doi.org/10.1103/PhysRevD.53.2610
99. S.J. Baker, R.F. Bishop, N.J. Davidson, Nucl. Phys. B (Proc. Suppl.) **53**, 834 (1997). https://doi.org/10.1016/S0920-5632(96)00795-5
100. C. Zeng, D.J.J. Farnell, R.F. Bishop, J. Stat. Phys. **90**, 327 (1998). https://doi.org/10.1023/A:1023220222019
101. N.E. Ligterink, N.R. Walet, R.F. Bishop, Ann. Phys. (NY) **267**(1), 97 (1998). https://doi.org/10.1006/aphy.1998.5812
102. N.E. Ligterink, N.R. Walet, R.F. Bishop, Ann. Phys. (NY) **284**(2), 215 (2000). https://doi.org/10.1006/aphy.2000.6070
103. R.F. Bishop, N.J. Davidson, R.M. Quick, D.M. van der Walt, J. Chem. Phys. **113**(10), 4008 (2000). https://doi.org/10.1063/1.1285806
104. D.J.J. Farnell, R.F. Bishop, in *Quantum Magnetism*, vol. 645, Lecture Notes in Physics, ed. by U. Schollwöck, J. Richter, D.J.J. Farnell, R.F. Bishop (Springer, Berlin, 2004), pp. 307–348. https://doi.org/10.1007/BFb0119597
105. G. Hagen, T. Papenbrock, M. Hjorth-Jensen, D.J. Dean, Rep. Prog. Phys. **77**(9), 096302 (2014). https://doi.org/10.1088/0034-4885/77/9/096302
106. R.F. Bishop, P.H.Y. Li, R. Zinke, R. Darradi, J. Richter, D.J.J. Farnell, J. Schulenburg, J. Magn. Magn. Mater. **428**, 178 (2017). https://doi.org/10.1016/j.jmmm.2016.11.043
107. R.F. Bishop, P.H.Y. Li, O. Götze, J. Richter, Phys. Rev. A **100**, 024401 (2019). https://doi.org/10.1103/PhysRevB.100.024401
108. R.F. Bishop, H.G. Kümmel, Phys. Today **40**(3), 52 (1987). https://doi.org/10.1063/1.881103
109. G. Rempe, H. Walther, N. Klein, Phys. Rev. Lett. **58**, 353 (1987). https://doi.org/10.1103/PhysRevLett.58.353
110. J.S. Arponen, R.F. Bishop, E. Pajanne, N.I. Robinson, Phys. Rev. A **37**, 1065 (1988). https://doi.org/10.1103/PhysRevA.37.1065
111. N. Bogolubov, J. Phys. USSR **11**, 23 (1947). https://www.ufn.ru/pdf/jphysussr/1947/11_1/3jphysussr19471101.pdf
112. E.P. Gross, Nuovo Cim. **20**, 454 (1961). https://doi.org/10.1007/BF02731494
113. L.P. Pitaevskii, Zh. Eksp. Teor. Fiz. **40**, 646 (1961). http://www.jetp.ac.ru/cgi-bin/e/index/e/13/2/p451?a=list. [translated into English in Sov. Phys. JETP **13**, 451–454 (1961)]
114. E. Seidewitz, Found. Phys. **47**, 355 (2017). https://doi.org/10.1007/s10701-017-0065-8
115. F. Constantinescu, E. Magyari, *Problems in Quantum Mechanics* (Pergamon, Oxford, 1971). https://www.elsevier.com/books/problems-in-quantum-mechanics/constantinescu/978-0-08-019008-2
116. A. Messiah, *Quantum Mechanics* (Dover Publ. Inc., Mineola, NY, 2014). https://store.doverpublications.com/048678455x.html
117. J.J. Sakurai, J. Napolitano, *Modern Quantum Mechanics*, 2nd edn. (Cambridge University Press, 2017). http://www.cambridge.org/gb/academic/subjects/physics/quantum-physics-quantum-information-and-quantum-computation/modern-quantum-mechanics-2nd-edition#tcu7XVr4RT24xaIM.97
118. S. Tomonaga, Prog. Theor. Phys. **1**, 27 (1946). https://doi.org/10.1143/PTP.1.27
119. J. Schwinger, Phys. Rev. **74**, 1439 (1948). https://doi.org/10.1103/PhysRev.74.1439
120. F.J. Dyson, Phys. Rev. **75**, 486 (1949). https://doi.org/10.1103/PhysRev.75.486