Koopman wavefunctions and classical-quantum correlation dynamics

Denys I. Bondar

Department of Physics and Engineering Physics, Tulane University, New Orleans, USA

François Gay-Balmaz

CNRS and École Normale Supérieure, Laboratoire de Météorologie Dynamique, Paris, France

Cesare Tronci

Department of Mathematics, University of Surrey, Guildford, UK and Mathematical Sciences Research Institute, Berkeley CA, USA

Upon revisiting the Hamiltonian structure of classical wavefunctions in Koopman-von Neumann theory, this paper addresses the long-standing problem of formulating a dynamical theory of classical-quantum coupling. The proposed model not only describes the influence of a classical system onto a quantum one, but also the reverse effect – the quantum backreaction. These interactions are described by a new Hamiltonian wave equation overcoming shortcomings of currently employed models. It is shown that the density matrix of the quantum subsystem is always positive, while the Liouville density of the classical subsystem may become negative. The proposed hybrid description is illustrated on the exactly solvable example of a degenerate two-level quantum system coupled to a classical harmonic oscillator.

SIGNIFICANCE STATEMENT

Since the dawn of quantum mechanics a Hamiltonian description for the interaction between quantum and classical systems has been sought, however with limited success. We finally furnish such a model that overcomes shortcomings of previous attempts. This finding may open new venues in the foundation of quantum mechanics as well as enable the development new generation computational methods in quantum chemistry.

INTRODUCTION

Classical-quantum coupling has been an open problem since the rise of quantum mechanics. Bohr’s concept of uncontrollable disturbance [5] affecting both classical and quantum systems during the measurement process has attracted much attention over the decades and it would be unfeasible to provide here the enormous list of works in this field. The effect of the uncontrollable disturbance on the quantum system is often known under the name of ‘decoherence’ [64] and it manifests in terms of non-unitary dynamics and purity non-preservation [61]. Recently the dynamics of a classical measuring device interacting with a quantum system has become a subject of experimental investigations (see, e.g., [29]). Over the last four decades, the apparent impossibility of a fully deterministic Hamiltonian description of classical-quantum coupling has been overcome by modeling decoherence in terms of Markov stochastic processes. Then, the quantum Lindblad equation [24, 38] has emerged as the most general type of a Markovian master equation describing the evolution of a positive-definite and unit-trace quantum density matrix. Lindblad’s theory, however, does not comprise the dynamics of the classical subsystem, which is simply treated as a thermodynamical bath.

In many physical contexts (in e.g., quantum chemistry and laser cooling), the systems under consideration are to be modeled as hybrid evolution to capture the coupling between electronic degrees of freedom and heavy nuclei. Then, it becomes essential to capture the ‘quantum backreaction’ – the quantum feedback force on the evolution of the classical system (i.e., the nuclei). To this purpose, in 1981 Aleksandrov [1] and Gerasimenko [22] independently proposed the following quantum-classical Liouville equation for an operator-valued density on phase-space \( \mathcal{D}(q, p, t) \):

\[
\frac{\partial \mathcal{D}}{\partial t} = -i\hbar^{-1}[\hat{H}, \mathcal{D}] + \frac{1}{2} \left( \{\hat{H}, \mathcal{D}\} - \{\mathcal{D}, \hat{H}\} \right),
\]

where \( \hat{H}(q, p) \) is the operator-valued Hamiltonian function and we have used the standard notation for commutators \([,\] and canonical Poisson brackets \(\{,\}\). This work by Aleksandrov and Gerasimenko has been highly influential and its Wigner-transformed variant is currently used for modeling purposes [33]. Shortly after its appearance, the Aleksandrov-Gerasimenko (AG) equation (1) was rediscovered in [9], where it was derived from first principles in terms of invariance properties under canonical and unitary transformations. However, although equation (1) conserves the total energy \( h = \text{Tr} \int \hat{H} \mathcal{D} \, dq \, dp \), the quantum density matrix \( \int \mathcal{D} \, dq \, dp \) is not positive definite. More importantly, the AG equation lacks a Hamiltonian structure and this is due to the fact that the binary operation in the right-hand side of (1) does not sat-
isfy the Jacobi identity and thus it is not a type of Poisson bracket \[11, 45, 52\]. Since the isolated classical and quantum dynamics both have Hamiltonian descriptions, it is natural to expect that the classical-quantum hybrid should inherit the same structure. Despite several efforts \[2, 13, 17, 18, 28, 46, 48, 49, 53\], Lie-algebraic arguments \[11\] tend to exclude the existence of a closed equation for \(\mathcal{D}\) possessing a Hamiltonian structure (i.e. comprising the Jacobi identity).

Another stream of research on classical-quantum coupling goes back to Sudarshan’s measurement theory \[54\] of 1976. Therein, Sudarshan proposed to couple classical and quantum dynamics by exploiting the Koopman-von Neumann (KvN) formulation of classical dynamics in terms of classical wavefunctions \[36, 62\]. Rediscovered in several instances \[16, 58\], this reformulation of classical mechanics has been attracting increasing attention \[8, 23, 35, 41, 47, 60, 63\]. See also \[10\] for a broad review of general applications of Koopman operators. In the KvN construction, the classical Liouville density \(\rho(q, p, t)\) is expressed as \(\rho = |\Psi|^2\), where \(\Psi(q, p, t)\) is a wavefunction obeying the KvN equation

\[
\frac{i}{\hbar} \frac{\partial \Psi}{\partial t} = \{i H, \Psi\} =: \hat{L}_H \Psi .
\]  

Here, we have introduced the Hermitian Liouvillian operator \(\hat{L}_H = iH\{H, \cdot\}\). A direct verification shows that the prescription \(\rho = |\Psi|^2\) returns the classical Liouville equation \(\partial_t \rho = \{H, \rho\}\). Upon working in the Heisenberg picture, Sudarshan extended the above equation (2) to include the interaction with quantum degrees of freedom by invoking special superselection rules to enforce physical consistency \[54\]. Although extremely inspiring, this approach has received some criticism over the years \[3, 44, 55, 56\] mainly because the role of the superselection rules remains somewhat unclear. Still, one of the advantages of Sudarshan’s proposal is that Koopman wavefunctions possess a simple canonical Hamiltonian structure formally equivalent to that underlying Schrödinger’s equation. Indeed, this feature provides a great simplification over the AG approach, which instead is based on density operators and Wigner functions both carrying highly noncanonical Lie-Poisson brackets \[4\].

While several hybrid theories appearing in the literature may offer good approximations of classical-quantum coupling, a Hamiltonian theory is still lacking and this poses specific problems concerning consistent transformation properties. This Letter addresses this problem by following up on Sudarshan’s idea of exploiting classical wavefunctions. Upon combining this approach with Hamiltonian methods, we shall show that KvN theory can be easily extended in such a way that its Hamiltonian functional coincides with the physical energy. In the second part of the paper we shall infer a Hamiltonian theory for classical-quantum coupling by using the extended KvN representation within the context of geometric quantization. The proposed classical-quantum wave equation is illustrated on the exactly solvable model of a degenerate two-level quantum system quadratically coupled to a one-dimensional classical harmonic oscillator.

**KOOPMAN WAVEFUNCTIONS**

We begin by looking at the Hamiltonian structure of the KvN equation (2). This structure is particularly transparent when looking at its variational formulation

\[
\delta \int_{t_1}^{t_2} \left( \hbar \text{Re}(\Psi^* \partial_t \Psi) - \Psi^* \hat{L}_H \Psi \right) d^6 z dt = 0 , \tag{3}
\]

which leads to a few observations.

First, the Hamiltonian functional for the KvN equation (2) is written as \(h = \int \Psi^* L_H \Psi d^6 z = \hbar \int \text{Im} \{\Psi^* , \Psi\} d^6 z\), where we have denoted \(z = (q, p)\). Then, we observe that the Hamiltonian functional for the KvN equation does not coincide with the total physical energy, which instead would read \(\int H |\Psi|^2 d^6 z\) (according to the prescription \(\rho = |\Psi|^2\)).

The second observation is that the quantity \(\text{Im} \{\Psi^*, \Psi\}\) satisfies the classical Liouville equation and thus, in principle we could set \(\rho = \text{Im} \{\Psi^*, \Psi\}\). Borrowing a terminology from fluid dynamics \[14\], this expression is often known as a Clebsch representation \[30, 40, 42\] in the context of Geometric Mechanics \[31, 39\]. However, here we are left with the insurmountable problem that \(\int \text{Im} \{\Psi^*, \Psi\} d^6 z = 0\).

The third observation is more fundamental: we remark that the KvN Lagrangian (the integrand in (3)) does not transform consistently under local phases. However, this problem can be overcome by using the minimal coupling method in gauge theory. Let us introduce the multiplicative operator \(\tilde{Z} = z\) and its canonical conjugate \(\tilde{\Lambda} = -i \hbar \nabla\), and let us rewrite the Liouvillian as \(\hat{L}_H = X_H(\tilde{Z}) \cdot \tilde{\Lambda}\). Here, \(X_H = J^\dagger H\) is the classical Hamiltonian vector field and \(J\) is (the inverse of) the canonical symplectic form, so that \([\tilde{Z}^i, \tilde{\Lambda}^j] = i \hbar \delta^{ij}\). Then, if \((\Phi, \mathcal{A})\) are the components of a \(U(1)\)-gauge potential, a gauge-covariant Lagrangian is constructed by the replacement

\[
X_H(\tilde{Z}) \cdot \tilde{\Lambda} \longrightarrow \Phi(\tilde{Z}) + X_H(\tilde{Z}) \cdot (\tilde{\Lambda} - \mathcal{A}(\tilde{Z})). \tag{4}
\]

Now, the choice of gauge potential is prescribed in prequantization theory \[21, 59\] as follows:

\[
\Phi(z) = H(z) , \quad \mathcal{A}(z) \cdot dz = \frac{1}{2} Jz \cdot dz . \tag{5}
\]

Under the replacement (4), the variational principle (3) yields the modified KvN equation

\[
\frac{i}{\hbar} \frac{\partial \Psi}{\partial t} = \{i H, \Psi\} - \left( \frac{1}{2} z \cdot \nabla H - H \right) \Psi =: \hat{\tilde{L}}_H \Psi . \tag{6}
\]
This equation already appeared in previous works \cite{9, 32, 35}, where it was noted that the expression \( \rho = |\Psi|^2 \) again satisfies the classical Liouville equation. Although here we adopt the gauge (5), we remark that some authors \cite{9, 35} prefer the choice \( \mathcal{A} \cdot d\mathbf{z} = p \cdot dq \); in this gauge, the phase term in equation (6) is readily seen to coincide with the Lagrangian \( \mathcal{L} = p \cdot \partial_t H - H \), thereby reminding the important relation between phases and Lagrangians going back to Feynman’s thesis \cite{19}. Recently, the crucial role of both classical and quantum phases was also exploited in connection to the Hamilton-Jacobi theory \cite{50, 51}, although in that context the wavefunction is defined only on the position space.

First appeared in van Hove’s prequantization theory \cite{59}, the modified Liouvillian \( \hat{\mathcal{L}}_H \) is known as a \textit{prequantum operator} \cite{27} and it satisfies the Lie algebra relation \( [\hat{\mathcal{L}}_H, \hat{\mathcal{L}}_K] = i\hbar \mathcal{J}_{(H,K)} \). In addition, we have a one-to-one correspondence between the Hamiltonian \( H \) and the Hermitian operator \( \hat{\mathcal{L}}_H \) (unlike the correspondence \( H \mapsto \hat{\mathcal{L}}_H \), which is many-to-one). In the Heisenberg picture (here denoted by the superscript \( \text{H} \)), one has \( d\hat{\mathcal{L}}_H^\text{H}/dt = i\hbar^{-1}[\hat{\mathcal{L}}_H^\text{H}, \hat{\mathcal{L}}_K^\text{H}] = -\mathcal{J}^\text{H} \) so that \( \mathcal{J}^\text{H} = \{\mathcal{A}^\text{H}, H^\text{H}\} \). Here, we shall call (6) the Koopman-van Hove (KvH) equation and address the reader to \cite{32, 35} for more discussions on how prequantization relates to KvN theory.

Let us now examine the Hamiltonian structure of the modified KvN equation (6). The variational principle \( \delta \int_1^Z \left( \hbar \text{Re}(i\Psi^* \partial_t \Psi) - \Psi^* \delta \hat{\mathcal{L}}_H \Psi \right) d^6z \; dt = 0 \) determines the Hamiltonian functional

\[
 h = \int \Psi^* \hat{\mathcal{L}}_H \Psi \; d^6z = \int H(|\Psi|^2 + \text{div} \mathbf{J}) \; d^6z, \quad (7)
\]

with

\[
 \mathbf{J} = \Psi^* \hat{\mathbf{\nabla}} \Psi, \quad \text{and} \quad \hat{\mathbf{\nabla}} := \hat{\mathbf{\nabla}}_\pm := \hat{\mathbf{\nabla}}(\pm \mathbf{\nabla} - \mathcal{A}).
\]

We note in passing that the operators \( \hat{\mathbf{\nabla}}_\pm \) satisfy the commutation relations \( \left[ \hat{\mathbf{\nabla}}_+^\dagger, \hat{\mathbf{\nabla}}_- \right] = \mp i\hbar \mathbf{J}^\parallel \) and \( \left[ \hat{\mathbf{\nabla}}_+^\parallel, \hat{\mathbf{\nabla}}_-^\dagger \right] = 0 \), which were used in \cite{8, 15} to rewrite quantum theory in terms of wavefunctions on phase-space. From equation (7), we see that the quantity \( |\Psi|^2 + \text{div} \mathbf{J} \) emerges as an alternative Clebsch representation for the Liouville density. More specifically, this quantity is a momentum map \cite{25, 26, 31, 39} for the group of strict contact transformations generated by the operator \( i\hbar^{-1} \hat{\mathcal{L}}_H \) \cite{59}, where

\[
 \hat{\mathcal{L}}_H = H - \mathbf{\nabla} H \cdot \hat{\mathbf{\nabla}}_+.
\]

While some of this material is illustrated in the Appendix, we shall leave a more thorough discussion of these aspects for future work. Here we emphasize that the momentum map property enforces the quantity \( |\Psi|^2 + \text{div} \mathbf{J} \) to satisfy the classical Liouville equation, as can be verified by a direct and lengthy calculation.

At this point, given the expression of the total energy (7), we insist that this must be equal to the total physical energy \( \int H \rho \; d^6z \), and thus we are led to the identification

\[
 \rho = |\Psi|^2 + \text{div}(\Psi^* \hat{\mathbf{\nabla}}_+ \Psi). \quad (8)
\]

Although we observe that this expression for the Liouville density is not positive-definite, its sign is preserved in time since the Liouville equation is a characteristic equation. Remarkably, we notice that the term \( \text{div} \mathbf{J} \) does not contribute to the total probability, so that \( \int \rho \; d^6z = \int |\Psi|^2 \; d^6z = 1 \). On the other hand, the same divergence term does contribute to expectation values, so that e.g. \( \langle \mathbf{z} \rangle = \int \rho \; d^6z = \int \Psi^* \hat{\mathbf{\nabla}}_+ \Psi \; d^6z \). As shown in \cite{8}, this last relation returns the usual Ehrenfest equations for the expectation dynamics of canonical observables. Another feature of relation (8) is that the presence of first-order derivatives may allow for \( \delta \)-like singularities (point particle solutions), which instead are removed by the usual KvN prescription \( \rho = |\Psi|^2 \). Lastly, we remark that the entire discussion can be repeated by replacing classical wavefunctions with positive-definite density-like operators mimicking Von Neumann’s density matrix \cite{9}. Then, equation (6) is recovered upon setting \( \hat{\mathbf{D}}(\mathbf{z}, \mathbf{z}', t) = \Psi(\mathbf{z}, t) \Psi^*(\mathbf{z}', t) \) in the evolution equation

\[
 i\hbar \partial_t \hat{\mathbf{D}} = [\hat{\mathcal{L}}_H, \hat{\mathbf{D}}]. \quad (9)
\]

In the following Sections, we shall further extend the present gauge-covariant KvN construction to include the coupling to quantum degrees of freedom.

\section*{Hybrid Classical-Quantum Dynamics}

The formulation of hybrid classical-quantum dynamics is usually based on fully quantum treatments, in which some kind of factorization ansatz is invoked on the wave function. This ansatz is then followed by a classical limit on the factor that is meant to model the classical particle.

Here, we propose a different perspective: we shall start with the KvH construction for two classical particles and we shall perform a formal quantization procedure on one of them. In geometric quantization \cite{27, 37}, one starts with the KvH equation (6) with \( \mathcal{A} = p \cdot dq \) and \( H = p^2/2m + V(q) \). Then, one enforces the polarization condition \( \partial_p \Psi = 0 \) and replaces \( p \Psi \) by \(-i\hbar \partial_q \Psi \). Eventually, one is left with Schrödinger’s equation. Although this process is the subject of current studies involving a more general type of Hamiltonian \( H \), here we shall proceed at a purely formal level.

At this point, we may obtain a hybrid classical-quantum theory by adopting a partial quantization procedure, as already suggested by Gerasimenko \cite{22} in the context of Weyl quantization. Consider the
the following classical-quantum wave equation for the hybrid wavefunction (here, denoted by \( \Upsilon(z, x) \)):

\[
\mathbf{i} \hbar \partial_t \Upsilon = \hat{H} \Upsilon - \nabla \hat{H} \cdot \mathbf{\hat{Z}}_z \Upsilon =: \hat{\mathcal{L}}_{\hat{H}} \Upsilon ,
\]

(10)

where

\[
\hat{H} = -\frac{\hbar^2}{2M} \Delta_x + \frac{1}{2M} p^2 + V(q, x)
\]

(11)

and we have defined the hybrid Liouvillian \( \hat{\mathcal{L}}_{\hat{H}} = \hat{H} - \nabla \hat{H} \cdot \mathbf{\hat{Z}}_z \).

Equations with a similar structure were shown to occur in the Hamiltonian dynamics of quantum expectation values [6, 7]. More importantly, equations precisely of the type (10) were considered in [9]. However, in that paper the authors rejected such equations because of interpretative questions mainly emerging from the fact that the role of the operator \( \hat{\mathcal{L}}_{\hat{H}} \) was somewhat unclear. For example, in [9] the authors claimed that (10) (or its analogue for \( \Upsilon(z, x) \Upsilon^\dagger(z', x') \)) does not conserve a positive energy. Here, we point out that, since \( \hat{\mathcal{L}}_{\hat{H}} \) is Hermitian, then (10) is actually a Hamiltonian equation possessing a variational principle of the type

\[
\delta \int_{t_1}^{t_2} \text{Re} \langle \Upsilon | (\mathbf{i} \hbar \partial_t - \hat{\mathcal{L}}_{\hat{H}}) \Upsilon \rangle \, dt = 0 ,
\]

(12)

thereby preserving the energy invariant

\[
h = \langle \Upsilon | \hat{\mathcal{L}}_{\hat{H}} \Upsilon \rangle = \text{Tr} \int \Upsilon^\dagger(z) \hat{\mathcal{L}}_{\hat{H}} \Upsilon(z) \, d^6z .
\]

(13)

Here, dagger denotes the adjoint in the quantum coordinates and similarly for the trace, so that \( \langle \Upsilon_1 | \Upsilon_2 \rangle = \text{Tr}(\Upsilon_1^\dagger \Upsilon_2) \).

Now we construct a generalized density operator \( \hat{D} \) so that the total energy (13) reads \( h = \text{Tr} \int \hat{H} \hat{D} \, d^6z \). Actually, the latter relation is obtained by a direct manipulation of the expression (13), upon defining

\[
\hat{D}(z) = \Upsilon(z) \Upsilon^\dagger(z) + \text{div}(\Upsilon(z) \mathbf{\hat{Z}}_z \Upsilon^\dagger(z)) .
\]

(14)

This quantity plays the role of the AG generalized density in (1) and it belongs to the dual of the tensor product space of phase-space functions and Hermitean operators on the quantum state space. Since the latter tensor space is not a Lie algebra (notice \( [\hat{\mathcal{L}}_F, \hat{\mathcal{L}}_G] \neq \hat{\mathcal{L}}_R \) for some \( \hat{\mathcal{L}}_z \)), \( \hat{D} \) does not carry momentum map properties and thus it cannot possess a closed Hamiltonian equation, in agreement with [11].

In addition, we remark that \( \hat{D} \) is generally not positive definite and, unlike the purely classical case, its sign is not preserved in time. This feature (also occurring in the AG equation (1)) was justified in [9] by analogies with Wigner quasi-probability densities. In the present context, the quantum density matrix and the classical Liouville density read

\[
\dot{\rho} = \int \hat{D}(z) \, d^6z = \int \Upsilon(z) \Upsilon^\dagger(z) \, d^6z .
\]

(15)

\[
\rho(z) = \text{Tr} \hat{D}(z) = \text{Tr} \left[ \Upsilon(z) \Upsilon^\dagger(z) + \text{div}(\Upsilon(z) \hat{\mathbf{Z}}_z \Upsilon^\dagger(z)) \right] .
\]

(16)

Then, while the quantum density matrix is positive definite by construction (unlike the AG theory [1, 22]), the classical Liouville density is allowed to become negative during the classical-quantum interaction.

A further consequence of equation (10) is obtained by simply applying Ehrenfest’s theorem: indeed, the case \( \hat{\mathcal{L}}_{\hat{H}} = 0 \) for some \( \hat{\mathcal{L}} = \mathbf{i} \hbar \nabla \mathbf{z} \) obviously recovers conservation of total momentum for Hamiltonians of the type (11). We remark that the expectation dynamics (17) differs from the corresponding result obtained from the AG equation (1).

We conclude by presenting the dynamics of \( \hat{D} \). As we pointed out, \( \hat{D} \) does not possess a closed Hamiltonian equation: this means that its evolution can only be expressed in terms of \( \Upsilon \). In the case of a finite-dimensional quantum state space, a lengthy computation shows that (in index notation)

\[
\partial_t \hat{D}_{\alpha\beta} = -\mathbf{i} \hbar^{-1} \left[ \hat{H}, \hat{D} \right]_{\alpha\beta} + \left[ \hat{H}, \hat{\mathcal{L}}_{\hat{H}} \right]_{\alpha\beta} + \mathbf{i} \hbar^{-1} \text{div} \left( \frac{\mathbf{z}}{2} \cdot \nabla \hat{H}, \frac{\mathbf{z}}{2} \Upsilon^\dagger \Upsilon \right)_{\alpha\beta}
\]

\[
- \left( \hat{H} - \frac{\mathbf{z}}{2} \cdot \nabla \hat{H}, \Upsilon \Upsilon^\dagger \right)_{\alpha\beta} - \frac{\mathbf{z}}{2} \cdot \nabla \hat{H}, \Upsilon \Upsilon^\dagger \right)_{\alpha\beta}
\]

\[
- \left( \frac{\mathbf{z}}{2} \cdot \nabla \hat{H}_{\gamma\delta}, \Upsilon_{\gamma\delta} \right)_{\alpha\beta} - \frac{\mathbf{z}}{2} \cdot \nabla \hat{H}_{\gamma\delta}, \Upsilon_{\gamma\delta} \right)_{\alpha\beta}
\]

\[
+ \mathbf{i} \hbar \left\{ \hat{H}_{\alpha\gamma}, \Upsilon_{\gamma\delta} \right\} \Upsilon_{\delta} - \mathbf{i} \hbar \left\{ \Upsilon_{\gamma\delta}, \hat{H}_{\gamma\delta} \right\} \Upsilon_{\delta} ,
\]

(18)

where all quantities are evaluated at \( z \). Despite the striking similarity between the first line above and Aleksandrov’s equation (1), the remaining terms in the \( \hat{D} \)-equation show that the classical-quantum interaction may be more involved than one might have expected. Nevertheless, the intricate nature of classical-quantum coupling becomes hidden by the formal simplicity of the following equations for the
quantum and classical densities:

\[ i\hbar \partial_t \hat{\rho} = \int \{\hat{H}, \hat{D}\} d^6z, \quad \partial_t \rho = \text{Tr}(\hat{H}, \hat{D}) , \] (19)

which coincide formally with the corresponding result obtained by using the AG equation (1).

We remark that none of the results discussed here require the specific form (11) of the hybrid Hamiltonian, which on the other hand was needed in first instance for the consistent derivation of the classical-quantum wave equation (10) by exploiting geometric quantization.

**Discussion**

Quantum decoherence emerges from purity non-preservation as it arises from the first in (19). Also, we observe that classical dynamics can be different from what we are used to in the absence of classical-quantum interaction. First, the last equation in (19) does not generally allow for point particle solutions. Since the latter are known to be classical pure states [12, 53], we conclude that classical-quantum correlations induce a loss of classical purity that mimics quantum decoherence effects. This will be illustrated below on an exactly solvable example.

Second, as we pointed out, positivity of \( \rho \) is not preserved in time [9]. Although this may seem surprising at first, an analogue of this situation can be readily found in the standard case of a harmonic oscillator interacting (by a linear or quadratic coupling) with a nonlinear quantum system. Let us consider the full quantum case in the Wigner representation: the Wigner-Moyal equation for \( W(z, \zeta) \) reads

\[ \partial_t W = \{\{ H, W \} \}, \] (20)

where the Poisson bracket \( \{ \cdot, \cdot \} \) denotes the Moyal bracket in the set of coordinates given by the subscript. Here, \( H(z, \zeta) \) is quadratic in \( z \), so that \( \{\{ H, W \} \} = \{ H, W \} \), while it retains arbitrary nonlinear dependence on \( \zeta \). We emphasize that, in the absence of the nonlinear quantum system, \( \nabla_\zeta H = 0 \) and the oscillator undergoes classical evolution (while its quantum features are encoded in the initial condition) and the coupled system can be considered as equivalent to a hybrid system. Then, projecting out the quantum coordinates yields the following equation for \( \varrho(z) = \int W(z, \zeta) d^6\zeta \):

\[ \partial_t \varrho = \int \{ H, W \} d^6\zeta , \] (21)

which is exactly the analogue of our second equation in (19). Also in this case, even if \( \varrho > 0 \) initially, despite the classical structure of the oscillator subsystem, its density \( \varrho \) may develop negative values in time because \( W \) is not generally positive. Then, as already pointed out by Feynman [20], the possibility of non-positive classical distributions in compound systems does not come as a surprise. Further discussions on the meaning of negative probabilities and their applications can be found, e.g., in [20, 34].

In addition, we wish to emphasize that, similarly to the AG theory in [1, 22] and unlike Sudarshan’s model [54], the present construction consistently recovers the mean-field model for the classical and quantum densities. This is readily verified by replacing the mean-field factorization ansatz \( \Psi(z, x) = \Psi(z)\psi(x) \) in the variational principle (12). Indeed, this operation returns

\[ i\hbar \partial_t \Psi = \{\psi| \hat{H} \psi\} \Psi - \nabla\langle \psi| \hat{H} \psi \rangle \cdot \hat{E}_x \Psi \] (20)

\[ i\hbar \partial_t \psi = \left( \int \Psi^\star \hat{E}_z \Psi d^6z \right) \psi , \] (21)

so that the equations for the quantum density \( \hat{\rho} = \psi \psi^\dagger \) and the classical distribution \( \rho \) (as given in (8)) return the mean-field equations in the form

\[ \partial_t \rho = \{\text{Tr}(\hat{\rho} \hat{H}), \rho\} , \quad i\hbar \partial_t \hat{\rho} = \left[ \int \rho \hat{H} d^6z , \hat{\rho} \right] . \] (22)

Notice that the above mean-field equations are recovered from (10) independently of the specific form of the hybrid Hamiltonian \( \hat{H}(z) \) and this leads us to extend the classical-quantum wave-equation (10) to apply for arbitrary types of Hamiltonians.

Before concluding this section, it may be relevant to highlight that the whole construction presented here can also be reformulated in terms of a density-like operator, by following Boucher and Traschen [9]. Indeed, one can simply replace the classical-quantum wave equation (10) by its correspondent for a positive-definite density-like operator \( \hat{\Theta} \), that is

\[ i\hbar \partial_t \hat{\Theta} = \left[ \hat{E}_z , \hat{\Theta} \right] , \] (23)

which we shall call classical-quantum von Neumann equation. Given the level of difficulty of such an extension of the theory, in this paper we choose to leave this direction open for future work.

**Illustrative Example**

To demonstrate how the hybrid evolution develops quantum-classical correlations, we consider the case of a degenerate two-level quantum system quadratically coupled to a one-dimensional classical harmonic oscillator. The Hamiltonian of this system reads

\[ \hat{H} = H_0 + \frac{q^2}{2} \alpha \cdot \hat{\sigma} , \quad H_0 = \frac{p^2}{2m} + m\omega^2 \frac{q^2}{2} , \] (23)

where \( m \) and \( \omega \) denote respectively the mass and frequency of the harmonic oscillator, \( \hat{\sigma}_j \) are the Pauli
matrices \((j = 1, 2, 3)\) representing the two-level quantum system, and the vector \(\alpha\) comprises the classical-quantum coupling constants \(\alpha_j\). The hybrid equation of motion (10) reads in this case

\[
\frac{\partial \Upsilon}{\partial t} = \left[ q (m \omega^2 + \alpha \cdot \sigma) \frac{\partial}{\partial p} - \frac{p}{m} \frac{\partial}{\partial q} \right] \Upsilon, \tag{24}
\]

where \(\Upsilon = (\Upsilon_1(q, p, t), \Upsilon_2(q, p, t))^T \in \mathbb{C}^2\). The equations for each component are decoupled after introducing the wavefunction \(\Upsilon = \hat{U} \Upsilon\), where the unitary matrix \(\hat{U}\) is defined by \(\hat{U}(\alpha \cdot \sigma) \hat{U}^\dagger = \text{diag}(\lambda_1, \lambda_2)\). Then, solving each linear characteristic equation for \(\Upsilon_k\) leads to the following exact solution of (24), expressed in terms of the initial condition \(\Upsilon_k(t = 0)\):

\[
\Upsilon_1 = y_1(2) + |U_{11}|^2 [y_1(1) - y_1(2)] + U_{11}^* U_{12} [y_2(1) - y_2(2)], \tag{25}
\]

\[
\Upsilon_2 = y_2(1) + |U_{22}|^2 [y_2(2) - y_2(1)] + U_{12}^* U_{11} [y_1(1) - y_1(2)], \tag{26}
\]

where

\[
y_k(l) = \Upsilon_k \left( q = r_l \sin(\phi_l - t \sqrt{\omega_m}/m)/\sqrt{\omega_m}, p = r_l \cos(\phi_l - t \sqrt{\omega_m}/m), t = 0 \right), \tag{27}
\]

along with \(\omega_m = m \omega^2 + \lambda_l\) (we assume \(\lambda_l > 0\)), \(r_l = \sqrt{r^2 + m \omega q^2}\), and \(\phi_l = \text{Arg}(p + i \sqrt{m \omega q})\). Here, \(U_{kl}\) denotes the components of \(\hat{U}\) and \(\text{Arg}(x + iy)\) denotes the argument function on complex numbers.

Figure 1 depicts the classical-quantum evolution for such a system with the initial condition

\[
\Upsilon(t = 0) = \sqrt{\frac{\omega}{2\pi}} \frac{1 - (1 + \beta H_0) e^{-\beta H_0}}{\beta H_0^2} \begin{pmatrix} 1 \\ 0 \end{pmatrix} \tag{28}
\]

corresponding to the uncorrelated quantum-classical state, where the quantum state (15) is the ground (i.e., “up”) state and the classical Liouville density (16) is the Boltzmann state \(\rho \propto e^{-\beta H_0}\) with an inverse thermodynamic temperature \(\beta\) and \(H_0\) as given in (23). The long-tailed wavefunction \(\Psi\) given by the square root in (28) and corresponding to the classical Boltzmann state can be easily obtained upon recalling (8) and by solving the differential equation \(|\Psi|^2 + \text{div}(\Psi^* \nabla \Psi) = \omega \rho^\dagger \Psi^2 /2\pi\). The latter is taken into a linear first-order term for \(|\Psi|^2\) by changing to polar coordinates after setting a zero phase. We remark that the initial condition (28) represents a stationary state for the uncoupled classical-quantum system, that is \(\alpha = 0\).

Figure 1 uses the atomic units (a.u.), where the electron mass, the electron charge, and \(h\) are all set to a unity [65]. As it can be seen, the quantum-classical correlations rapidly develop yielding non-Gaussian classical Liouville densities (16) (due to the quantum backreaction) and non-pure quantum states (f). In other words, the classical system induces quantum decoherence [see figure 1(f)]. It is noteworthy that the classical density is non-negative for all times in the considered example.

Notice that the parameters chosen for figure 1 are such that \(\beta \gg 2/(\hbar \omega)\) implying that the initial condition (28) involves a cold classical state, whose phase space distribution in figure 1(a) violates the
Heisenberg uncertainty principle. Therefore, figure 1 displays truly hybrid dynamics, rendering quantum-classical correlations, that cannot be modeled by the Pauli equation. On the other hand, if we set $\beta = 2/(\hbar \omega)$, the classical Liouville density coincides at all times with the Wigner function for the Pauli spinor wavefunction $\psi(q) \propto e^{-m \omega q^2/(2\hbar)}(1, 0)^T$. For such an initial condition, the dynamics of the hybrid equation of motion (24) coincides with the Pauli equation with quantum Hamiltonian $\hat{p}^2/(2m) + m \omega^2 \hat{q}^2/2 + \alpha \hat{s} \hat{q}^2/2$, where $[\hat{q}, \hat{p}] = i\hbar$. This correspondence is another evidence for the reliability of the classical-quantum wave equation (10).

CONCLUSIONS

Upon combining KvN classical mechanics with van Hove’s prequantization theory, we have provided the new representation (8) of the Liouville density in terms of Koopman-van Hove classical wavefunctions. Then, given the KvH equation (6) for two particles, a quantization procedure was applied to one of them thereby leading to the classical-quantum wave equation (10) for the hybrid wavefunction $\Psi(z, x)$. This construction leads naturally to the identification of a sign-indefinite operator-valued density (14) encoding classical-quantum correlations. In turn, the latter can be discarded by invoking the factorization ansatz $\mathcal{T}(z, x) = \Psi(z) \psi(x)$ recovering the celebrated mean-field model (22).

Equations (10), (14), (15), and (16) constitute a long sought Hamiltonian model for classical-quantum hybrid evolution. As shown, the density matrix of the quantum subsystem is always positive, while the Liouville density of the classical subsystem may, in general, become negative. The proposed hybrid description has been illustrated on an example of the exactly solvable model of a degenerate two-level quantum system quadratically coupled to a one-dimensional classical harmonic oscillator. In this case, the quantum backreaction leads to positive-definite, yet non-Gaussian classical distributions.

In future works, we plan to develop effective numerical schemes for the classical-quantum wave equation (10) to be able to assess its physical consequences in experimentally relevant scenarios. For example, the identification of hybrid classical-quantum thermal equilibria is an interesting question whose answer may open new perspectives in the statistical mechanics of hybrid classical quantum systems [43].

Acknowledgments. We are grateful to Darryl D. Holm for his valuable comments during the writing of this work. Special thanks go to Paul Skerritt for his keen insight into the identification of specific initial conditions for the classical wavefunction. Also, the authors are indebted to Dorje Brody, Maurice de Gosson, Hans-Thomas Elze, Viktor Gerasimenko, Raymond Kapral, Robert Littlejohn, Giuseppe Marmo, Milan Radonjić, and Lorenzo Salcedo for stimulating correspondence and inspiring discussions. D.I.B. is supported by Air Force Office of Scientific Research Young Investigator Research Program (No. FA9550-16-1-0254). F.G.B was partially supported by the grant ANR-14-CE23-0002-01. C.T. acknowledges financial support from the Leverhulme Trust Research Project Grant No. 2014-112, and from the London Mathematical Society Grant No. 31633 (Applied Geometric Mechanics Network). This material is partially based upon work supported by the NSF Grant No. DMS-1440140 while C.T. was in residence at MSRI, during the Fall 2018 semester.

Appendix A: KvH momentum map

In this Section, we show explicitly that the relation (8) identifies a momentum map for the infinitesimal action given by the operator $\hat{L}_H$. In Geometric Mechanics [31, 39], momentum maps [25, 26] represent a generalization of Noether’s theorem to canonical group actions that are not necessarily a symmetry of the system under consideration. In this context, the Noether charge is generalized to a momentum map that evolves under the coadjoint representation associated to the Lie group acting on the considered mechanical system.

Without entering further details, we define the momentum map on symplectic vector spaces as follows. Let $(V, \Omega)$ be a vector space with symplectic form $\Omega$, and let the latter be preserved by a $G$-group action on $V$. Then, the momentum map $J : V \mapsto \mathfrak{g}^\ast$ taking values in the dual space $\mathfrak{g}^\ast$ of the Lie algebra $\mathfrak{g}$ of $G$ is defined as

$$2(\mathbf{J}(v), \xi) := \Omega(\xi \mathcal{V}(v), v),$$

where $\xi \in \mathfrak{g}$, $\mathcal{V}$ denotes the infinitesimal action on $V$, and $\langle \cdot, \cdot \rangle$ is the real-valued duality pairing for $\mathfrak{g}$. In the special case when $\Omega$ is canonical, the momentum map $J(v)$ is generally called a Clebsch representation.

In our case, $V$ is the space of classical wavefunctions, the Lie algebra is the space $\mathfrak{g} = C^\infty(\mathbb{R}^6)$ of phase-space functions (endowed with the canonical bracket and the standard $L^2$—pairing), and the infinitesimal generator $\mathcal{V}_\xi(v)$ reads $-i\hbar^{-1} \hat{L}_H \Psi$. Then, using the Schrödinger (canonical) symplectic form $\Omega(\Psi_1, \Psi_2) = 2\hbar \text{Im} \int \mathcal{V}_1^*(z) \mathcal{V}_2(z) d^6z$, the definition of momentum map reads

$$\int H J(\Psi) d^6z = \int \mathcal{V}^* \hat{L}_H \Psi d^6z.$$
Therefore, we compute
\[
\int \Psi^* \hat{L}_H \Psi \, d^6 z = \int \Psi^* \left[ \{ i \hbar H, \Psi \} + \left( H - \frac{1}{2} \mathbf{z} \cdot \nabla H \right) \Psi \right] \, d^6 z \\
= \int \left[ |\Psi|^2 + \text{div} \left( \frac{i}{2} \mathbf{z} |\Psi|^2 \right) \right] \, d^6 z \\
+ i \hbar \{ \Psi, \Psi^* \} H \, d^6 z
\]

Now, we observe that
\[
i \hbar \{ \Psi, \Psi^* \} = -i \hbar \text{div}(\Psi^* J \nabla \Psi) = \text{div}(\Psi^* J \hat{\Lambda} \Psi)
\]
so that the momentum map reads
\[
J(\Psi) = |\Psi|^2 + \text{div} \left[ \Psi^* \left( \frac{i}{2} \hat{Z} + J \hat{\Lambda} \right) \Psi \right],
\]
thereby recovering the relation (8) as a Clebsch representation. By proceeding analogously, we notice that $|\Psi|^2$ is also a Clebsch representation generated by local phase transformations with infinitesimal action $\xi_V(v)$ given as $-i \hbar^{-1} \phi \Psi$ (where $\phi(z)$ is a real phase-space function).

Notice that, since $-i \hbar^{-1} \hat{L}_H$ is skew-Hermitian, the correspondence $H \mapsto -i \hbar^{-1} \hat{L}_H$ provides a Lie algebra homomorphism between phase-space functions and skew-Hermitian operators on classical wavefunctions. Then, the map $-i \hbar \Psi(\mathbf{z}) \Psi^*(\mathbf{z}') \mapsto \hat{J}(\Psi)$ emerges as the dual of this Lie algebra homomorphism, thereby ensuring infinitesimal equivariance of $\hat{J}(\Psi)$ and the consequent Poisson mapping property [31, 39]. Thus, this guarantees that the momentum map $\hat{J}(\Psi)$ obeys the classical Liouville equation. Again, without entering further details, here we only mention that the operator $-i \hbar^{-1} \hat{L}_H$ emerges as the infinitesimal generator of the action of a Lie group first discussed in Van Hove’s thesis [59], which is at the heart of classical mechanics. Under the name of “strict contact transformations”, this Lie group is a central extension of standard canonical transformations. This and related points will be discussed in more detail in future work.

Appendix B: Hybrid dynamics

In this Appendix, we provide calculational details of the discussion concerning classical-quantum hybrids. First, we shall show that the definition (14) leads to rewriting the total energy (13) as

\[
h = \text{Tr} \int \mathcal{Y}^\dagger(\mathbf{z}) \hat{L}_H \mathcal{Y}(\mathbf{z}) \, d^6 z = \text{Tr} \int \hat{H} \hat{D} \, d^6 z.
\]

Indeed, we verify this as follows:

\[
\begin{align*}
\text{Tr} \int \mathcal{Y}^\dagger \left[ \hat{H} - \nabla \hat{H} \cdot \left( \frac{i}{2} \hat{Z} + J \hat{\Lambda} \right) \right] \mathcal{Y} \, d^6 z \\
= \text{Tr} \int \left[ \mathcal{Y} \mathcal{Y}^\dagger \hat{H} + \text{div} \left( \frac{i}{2} \mathcal{Y} \mathcal{Y}^\dagger \hat{Z} \right) \right] \, d^6 z \\
- \text{Tr} \int \hat{H} \text{div}(\mathcal{Y} J \hat{\Lambda} \mathcal{Y}^\dagger) \, d^6 z
\end{align*}
\]

where all quantities are evaluated at $\mathbf{z}$ and we used

\[
i \hbar \text{Tr} \int \mathcal{Y}^\dagger(\mathbf{z}) \hat{D} \, d^6 z = i \hbar \text{Tr} \int \hat{H} \{ \mathcal{Y}, \mathcal{Y}^\dagger \} \, d^6 z
\]

In conclusion, we recover the definition (14).

Now we want to prove the $\hat{D}$–equation (18). For this purpose, we shall use the adjoint of equation (10), that is

\[
-\imath \hbar \partial_t \mathcal{Y}^\dagger(\mathbf{z}) = \mathcal{Y}^\dagger(\mathbf{z}) \hat{H}(\mathbf{z}) - (\hat{Z}_- \mathcal{Y}^\dagger(\mathbf{z})) \cdot \nabla \hat{H}(\mathbf{z}),
\]
which arises from the relation $(\hat{Z}_+ \mathcal{Y}(\mathbf{z}))^\dagger = \hat{Z}_- \mathcal{Y}^\dagger(\mathbf{z})$. At this point, we restrict to finite dimensions and, upon taking the time derivative of the definition (14), one obtains
\[ \partial_t \tilde{D}_{\alpha\beta} = \frac{d}{dt} \left( \hat{\gamma}_\alpha \hat{\gamma}_\beta + \frac{1}{2} \text{div} (z \hat{Y}_\alpha \hat{Y}_\beta^*) + i \{ \hat{Y}_\alpha, \hat{Y}_\beta^* \} \right) \]

\[ = -i \hbar^{-1} \left( \hat{H}_{\alpha\gamma} - \frac{1}{2} z \cdot \nabla \hat{H}_{\alpha\gamma} \right) \hat{Y}_\gamma \hat{Y}_\beta^* + \{ \hat{H}_{\alpha\gamma}, \hat{Y}_\gamma \} \hat{Y}_\beta^* \]

\[ + i \hbar^{-1} \hat{Y}_\alpha \hat{Y}_\gamma^* \left( \hat{H}_{\gamma\beta} - \frac{1}{2} z \cdot \nabla \hat{H}_{\gamma\beta} \right) - \hat{Y}_\alpha \{ \hat{Y}_\gamma, \hat{H}_{\gamma\beta} \} \]

\[ + \text{div} \left( \frac{z}{2} \left( -i \hbar^{-1} \left( \hat{H}_{\alpha\gamma} - \frac{1}{2} z \cdot \nabla \hat{H}_{\alpha\gamma} \right) \hat{Y}_\gamma \hat{Y}_\beta^* + \{ \hat{H}_{\alpha\gamma}, \hat{Y}_\gamma \} \hat{Y}_\beta^* \right) \right) \]

\[ + \text{div} \left( \frac{z}{2} \left( i \hbar^{-1} \hat{Y}_\alpha \hat{Y}_\gamma^* \left( \hat{H}_{\gamma\beta} - \frac{1}{2} z \cdot \nabla \hat{H}_{\gamma\beta} \right) - \hat{Y}_\alpha \{ \hat{Y}_\gamma, \hat{H}_{\gamma\beta} \} \right) \right) \]

\[ + i \hbar \left\{ -i \hbar^{-1} \left( \hat{H}_{\alpha\gamma} - \frac{1}{2} z \cdot \nabla \hat{H}_{\alpha\gamma} \right) \hat{Y}_\gamma + \{ \hat{H}_{\alpha\gamma}, \hat{Y}_\gamma \} \right\} \hat{Y}_\beta^* \]

\[ + i \hbar \left\{ \hat{Y}_\alpha \left( i \hbar^{-1} \hat{Y}_\gamma^* \left( \hat{H}_{\gamma\beta} - \frac{1}{2} z \cdot \nabla \hat{H}_{\gamma\beta} \right) - \{ \hat{Y}_\gamma, \hat{H}_{\gamma\beta} \} \right) \right\} \]

We recall that in the present notation all quantities are evaluated at \( z \), e.g. \( \hat{Y}^T \) stands for \( \hat{Y}(z) \hat{T}(z) \).

We expand the divergence \( \text{div}(\hat{H} - \nabla \hat{H} \cdot z/2, \hat{Y}^T \hat{T}/2) \) in the 4th and 5th lines and we use the Leibniz product rule and the Jacobi identity in the last two lines. Then, a few cancelations yield

\[ \partial_t \tilde{D}_{\alpha\beta} = -i \hbar^{-1} \left[ \hat{H}, \hat{Y}^T \right] + \left\{ \hat{H}, \hat{Y}^T + i \{ \hat{Y}, \hat{T}^T \}_{\alpha\beta} \right\} - \{ \hat{Y}^T + i \hat{H}, \hat{T} \}_{\alpha\beta} \]

\[ + \text{div} \left( \frac{z}{2} \left[ \hat{H}, \hat{Y}^T \right] \right)_{\alpha\beta} - \left\{ \frac{z}{2} \hat{Y}^T, \hat{H} \right\}_{\alpha\beta} + i \hbar^{-1} \frac{z}{2} \cdot \nabla \hat{H}, \frac{z}{2} \hat{Y}^T \right\}_{\alpha\beta} \]

\[ - \text{div} \left( \frac{z}{2} \left[ \hat{H}_{\alpha\gamma}, \hat{Y}_\beta^* \right] \hat{Y}_\gamma - \frac{z}{2} \{ \hat{Y}_\alpha, \hat{H}_{\gamma\beta} \} \hat{Y}_\gamma \right) - \hat{Y}_\gamma \left( \frac{z}{2} \cdot \nabla \hat{H}_{\alpha\gamma}, \hat{Y}_\beta^* \right) + \{ \hat{Y}_\alpha, \frac{z}{2} \cdot \nabla \hat{H}_{\gamma\beta} \} \hat{Y}_\gamma^* \]

\[ + \left[ \hat{H} - \frac{z}{2} \cdot \nabla \hat{H}, \{ \hat{Y}, \hat{T}^T \} \right]_{\alpha\beta} + \{ \hat{H}, \hat{T} \left\{ \hat{Y}, \hat{T}^T \right\} \}_{\alpha\beta} - \{ i \hbar \{ \hat{Y}, \hat{T}^T \}, \hat{H} \}_{\alpha\beta} \]

\[ - i \hbar \{ \hat{Y}_\alpha, \{ \hat{H}_{\alpha\gamma}, \hat{Y}_\beta^* \} \} + i \hbar \left\{ \{ \hat{Y}_\alpha, \hat{H}_{\alpha\beta} \}, \hat{T}_\gamma^* \right\} . \]

Upon expanding the divergences in the second line and by using \( \{ \hat{H}, \hat{z} \} = -i \nabla \hat{H} \), further use of the Leibniz product rule yields the equation (18).

At this stage, we can verify the relations (19) explicitly. We begin by proving the first in (19), that is by computing \( \int \partial_t \tilde{D} \, d^6 z \). This is easily done by using the relation

\[ \int \{ z \cdot \nabla \hat{H}_{\alpha\gamma}, \hat{Y}_\beta^* \} \hat{Y}_\gamma \, d^6 z - \int \{ \hat{Y}_\alpha, z \cdot \nabla \hat{H}_{\gamma\beta} \} \hat{Y}_\gamma^* \, d^6 z \]

\[ = - \int [ z \cdot \nabla \hat{H}, \{ \hat{Y}, \hat{T}^T \} ]_{\alpha\beta} \, d^6 z , \]

which indeed yields the first in (19).

Analogously, the second in (19) is recovered by computing \( \text{Tr} \partial_t \tilde{D} \). To this purpose, we find

\[ \{ z \cdot \nabla \hat{H}_{\alpha\gamma}, \hat{Y}_\alpha \} \hat{Y}_\gamma - \{ \hat{Y}_\alpha, z \cdot \nabla \hat{H}_{\alpha\gamma} \} \hat{Y}_\gamma^* \]

\[ = \text{Tr} \{ z \cdot \nabla \hat{H}, \hat{Y}^T \} \]

as well as

\[ \text{div} \left( z \{ \hat{Y}_\alpha, \hat{Y}_\gamma \} \hat{Y}_\gamma^* - z \{ \hat{Y}_\alpha, \hat{H}_{\alpha\gamma} \} \hat{Y}_\gamma^* \right) \]

\[ = \text{div} \left( z \text{Tr} \{ \hat{Y}, \hat{T}^T \} \right) \]

\[ = \text{div} \left( \text{Tr} \{ \hat{H}, z \hat{T}^T \} - \text{Tr} \{ \hat{H}, \hat{T}^T \} \right) \]

\[ = \text{Tr} \left( z \cdot \nabla \hat{H}, \hat{Y}^T \right) \]

\[ - \text{Tr} \{ \hat{H}, \text{div} \left( z \hat{T}^T \right) \} \]

Then, the second in (19) follows from the relations

\[ \text{Tr} \{ (\hat{D}, \hat{H}) - \{ \hat{H}, \hat{D} \} \} = 2 \text{Tr} \{ \hat{D}, \hat{H} \} \]

\[ = \text{Tr} \{ (\hat{H} - \nabla \hat{H} \cdot z/2), \hat{D} \} - \text{Tr} \{ \hat{D}, \hat{H} - \nabla \hat{H} \cdot z/2 \} \]

as well as from the Jacobi identity \( \left( \{ \hat{H}_{\alpha\gamma}, \hat{Y}_\beta^* \}, \hat{Y}_\gamma \right) - \{ \hat{Y}_\gamma, \{ \hat{Y}_\alpha, \hat{H}_{\alpha\beta} \} \} = \text{Tr} \{ \{ \hat{Y}, \hat{T}^T \}, \hat{H} \} \)
