# Non-Hamiltonian Quantum Mechanics. Relation between operator and wave schemes of motion

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The symplectic structure of Weinberg's formalism for nonlinear quantum mechanics is first unveiled and then generalized to introduce non-Hamiltonian quantum mechanics. By exploiting the correspondence between wave and matrix mechanics, a link between this generalization and a non-Hamiltonian commutator, proposed recently by this author, is found. The general correspondence between operator and wave formalisms in non-Hamiltonian quantum mechanics is exploited to introduce a quantum-classical theory of wave fields. This can be considered as a first step toward a deeper understanding of the relation between operator quantum-classical mechanics, introduced some time ago, and the original quantum-classical scheme of motion where wave functions are evolved in time and the classical degrees of freedom follows surface-hopping trajectories on single quantum states.

## I. INTRODUCTION

Recently, Weinberg proposed an algebraic generalization of quantum mechanics [1] in order to describe nonlinear effects[2]. His approach followed a line of research that investigates the relations between classical and quantum theories [3]. As of now, there is no experimental evidence of nonlinear effects in quantum mechanics or, better to say, the usual quantum linear formalism seems to be able to treat the known phenomenology.

Therefore, one might ask, if there is any reason, beyond pure speculation, that could drive researchers to devise generalizations of quantum mechanics. As a matter of fact, an important motivation is provided by the necessity of expressing theories by means of mathematical structures which allow calculations to be performed in practice. Actually, the advent of fast computers has changed forever the perspectives researchers have on theories. Computers elicited the idea that mathematical objects must be calculable in practice in order not to be void of scientific value. This point of view is clearly presented in Kohn's nobel lecture [4]. Considerations about the computational complexity of a given theory enter into the scientific assessment and into the creative process itself. Thus, modern-day researchers deal with theories which have the new scope of creating mathematical formalisms that are meant for effective computational use. Important examples are given by Density Functional Theory [4], the Renormalization Group Theory [5], and Lattice Field Theory [6]. A general strategy for obtaining such "calculable" theories consists in creating mathematical structures that modify the conditions that defines the problem to be solved (for example by releasing some constraints). In this way, the original problem is mapped into a new one, whose solutions can coincide numerically (i.e. within tolerable statistical uncertainties) with those of the original problem, if certain conditions are satisfied by the calculation.

One important example of this type of theories is given, within the field of molecular dynamics, by non-Hamiltonian formalisms [7]. Non-Hamiltonian theories may be created by starting from a Lie algebra and subsequently allowing the Jacobi relation to be violated [8]. In classical mechanics non-Hamiltonian formalisms are commonly used to impose thermodynamical constraints [9], such as a constant temperature [7], by means of a few additional degrees of freedom. Such non-Hamiltonian systems have additional variables with respect to the original Hamiltonian structure from which they are derived and, for this reason, are usually called extended systems. In quantum mechanics, non-Hamiltonian theory emerged for treating consistently problems where classical and quantum degrees of freedom are present because of certain approximations [10]. It has already been showed that such quantum-classical theories are a particular realization of a general non-Hamiltonian quantum commutator [11]. Such non-Hamiltonian commutators are built by generalizing the symplectic structure of the ordinary quantum commutator [11]. Given that Weinberg's formalism is symplectic, the same idea that was used in Ref. [11] can be applied in order to generalize Weinberg's approach by setting it into a non-Hamiltonian algebraic structure. This leads to another way of treating nonlinear effects in quantum mechanics which might turn out useful in the future. In fact, while in Weinberg's formalism nonlinear effects are introduced by modifying in a suitable manner the Hamiltonian, in the formalism here proposed this is not necessary and one can just modify the antisymmetric matrix entering in the definition of the non-Hamiltonian algebra. The consistency of the non-Hamiltonian theory here presented is proved by showing that the Heisenberg picture, corresponding to the non-Hamiltonian wave dynamics that generalizes Weinberg's formalism, is defined by means of the very same non-Hamiltonian commutator proposed by this author in a previous paper [11].

The foundation of a non-Hamiltonian generalization of quantum mechanics is also useful for describing quantum-classical systems. As a matter of fact, it has already been shown that quantum-classical brackets [10] are a partic-

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ular realization of non-Hamiltonian commutators [11]. Therefore, the non-Hamiltonian structure of quantum-classical dynamics could be exploited for introducing thermodynamic constraints [11] and for defining a rigorous statistical theory of quantum classical systems with holonomic constraints [12], along the lines of Ref. [13]. In this paper, a connection between the usual "Heisenberg-like" formulation of quantum-classical dynamics and a wave scheme of motion is first found and then exploited in order to introduce quantum-classical wave dynamics. The fact that the quantum-classical dynamics of operators can be recast into a quantum-classical wave-function formalism is a first step toward the comprehension of the relation between the theory of Refs. [10] with the original formulation of quantum-classical evolution by means of wave-functions and surface-hopping trajectories [14]. It is worth to remark that a re-formulation of quantum-classical dynamics is interesting not only for theoretical reasons but also because current numerical implementations of quantum-classical dynamics by means of operators [15] are limited to short-time dynamics because of statistical uncertainties growing with time. Thus, there are hopes that the quantum-classical wave formalism here presented could provide a route to solve such numerical problems. Future works will be devoted to this issue.

This paper is organized as follows. In Section II Weinberg's formalism is briefly reviewed by unveiling its symplectic structure. In Section III Weinberg's formalism is generalized by means of non-Hamiltonian brackets. Moreover, by exploiting the correspondence between wave and matrix mechanics, ultimately resting onto an operator identity [16], it is shown that the non-Hamiltonian wave formalism is dual to the non-Hamiltonian matrix mechanics, which has been proposed recently by this author by means of non-Hamiltonian commutators. In Section IV quantum-classical dynamics, expressed into a "Heisenberg-like" scheme of motion by means of a particular choice of non-Hamiltonian commutator, is transformed into a "Schrödinger-like" theory in terms of quantum-classical wave fields evolving in time. This correspondence is established by means of an operator identity illustrated in Appendix A. Section V is devoted to conclusions and perspectives.

## II. WEINBERG'S FORMALISM

Consider the wave fields $|\psi\rangle$ and $\langle\psi|$, where Dirac's braket notation is used to denote $\psi(r) \equiv \langle r|\psi\rangle$ and $\psi^*(r) \equiv \langle\psi|r\rangle$. Observables are defined by functions of the type

$$a = \langle\psi|\hat{A}|\psi\rangle \; , \tag{1}$$

where the operators are Hermitian, $\hat{A} = \hat{A}^\dagger$. The quantum commutator can be introduced in symplectic form by first defining the antisymmetric matrix

$$\boldsymbol{\mathcal{B}}^c = \begin{bmatrix} 0 & 1 \\ -1 & 0 \end{bmatrix} \; , \tag{2}$$

and then writing

$$\begin{aligned} [\hat{A}, \hat{B}] &= \begin{bmatrix} \hat{A} & \hat{B} \end{bmatrix} \cdot \boldsymbol{\mathcal{B}}^c \cdot \begin{bmatrix} \hat{A} \\ \hat{B} \end{bmatrix} \\ &= \hat{A}\hat{B} - \hat{B}\hat{A} \; . \end{aligned} \tag{3}$$

In Weinberg's formalism it is necessary to define Poisson brackets citecm in terms of the wave fields $|\psi\rangle$ and $\langle\psi|$. To this end, one can introduce the following "phase space" coordinate $\chi \equiv (|\psi\rangle, \langle\psi|)$, so that $\chi_1 = |\psi\rangle$ and $\chi_2 = \langle\psi|$, and then introduce Poisson brackets of observables as

$$\{a, b\} = \sum_{\alpha=1}^{2} \frac{\partial a}{\partial \chi_\alpha} \mathcal{B}^c_{\alpha\beta} \frac{\partial b}{\partial \chi_\beta} \; . \tag{4}$$

The bracket in Eq. (4) defines a Lie algebra and a Hamiltonian systems. Typically, the Jacobi relation is satisfied

$$\mathcal{J} = \{a, \{b, c\}\} + \{c\{a, b\}\} + \{b, \{c, a\}\} = 0 \; . \tag{5}$$

In order to obtain the usual quantum formalism, one can introduce the Hamiltonian function in the form

$$h(|\psi\rangle, \langle\psi|) \equiv h(\chi) = \langle\psi|\hat{H}|\psi\rangle \; , \tag{6}$$

where $\hat{H}$ is the Hamiltonian operator of the system under study. Equations of motion for the wave fields can be written in compact form as

$$\frac{\partial \chi}{\partial t} = -\frac{i}{\hbar}\{\chi, h(\chi)\} \; . \tag{7}$$

The compact form of Eq. (7) can be set into an explicit form as

$$\frac{\partial}{\partial t}|\psi\rangle = -\frac{i}{\hbar}\mathcal{B}^c_{12}\frac{\partial h}{\partial\langle\psi|} \tag{8}$$

$$\frac{\partial}{\partial t}\langle\psi| = -\frac{i}{\hbar}\mathcal{B}^c_{21}\frac{\partial h}{\partial|\psi\rangle} \; . \tag{9}$$

It is easy to see that, when the Hamiltonian function is chosen as in Eq. (6), Eqs. (7), or their explicit form (8-9), gives the usual formalism of quantum mechanics. It is worth to remark that in order not to alter gauge invariance, the Hamiltonian and the other observables must obey the homogeneity condition

$$h = \langle\psi|(\partial h/\partial\chi_2)\rangle = \langle(\partial h/\partial\chi_1)|\psi\rangle \; . \tag{10}$$

If one considers the time evolution of the density $\rho = \langle\psi|\hat{1}|\psi\rangle$, the following continuity equation is obtained

$$\frac{\partial \rho}{\partial t} = -\frac{\partial}{\partial \chi} \cdot J \; , \tag{11}$$

where the current, $J$, has been defined as

$$J = \frac{i}{\hbar}\begin{bmatrix} \mathcal{B}^c_{12} h|\psi\rangle \\ \langle\psi|h\mathcal{B}^c_{21} \end{bmatrix} \; . \tag{12}$$

Weinberg showed how the formalism above given can be generalized in order to describe nonlinear effects in quantum mechanics [1]. To this end, one must maintain the homogeneity condition, Eq. (10), on the Hamiltonian but relax the constraint which assumes that the Hamiltonian must be a bilinear function of the wave fields. Thus, the Hamiltonian can be a general function given by

$$\mathcal{H} = \sum_{i=1}^{n} \rho^{-i} \mathcal{H}_i \; , \tag{13}$$

where $n$ is arbitrary integer that fixes the order of the correction, $\mathcal{H}_0 = h$, and

$$\begin{aligned} \mathcal{H}_1 &= \rho^{-1} \int dr dr' dr'' dr''' \psi^*(r)\psi^*(r') \\ &\times \; G(r, r', r'', r''')\psi(r'')\psi(r''') \; , \end{aligned} \tag{14}$$

with analogous expressions for higher order terms.

Applications and thorough discussions of the above formalism can be found in Ref. [1].

## III. NON-HAMILTONIAN THEORY

Once Weinberg's formalism is expressed by means of the symplectic form proposed in the previous Section, it can be generalized very easily in order to obtain a non-Hamiltonian quantum algebra. To this end, one can substitute the antisymmetric matrix $\boldsymbol{\mathcal{B}}^c$ with another antisymmetric matrix $\boldsymbol{\mathcal{B}} = \boldsymbol{\mathcal{B}}(f(r);\chi)$, whose elements might be functions of the coordinates and of any observables obeying the homogeneity condition in Eq. (10). By means of $\boldsymbol{\mathcal{B}}$ a non-Hamiltonian bracket $\{\!\!\{\ldots,\ldots\}\!\!\}$ can be defined as

$$\{\!\!\{a, b\}\!\!\} \;=\; \sum_{\alpha=1}^{2} \frac{\partial a}{\partial \chi_\alpha} \mathcal{B}_{\alpha\beta}(f(r);\chi) \frac{\partial b}{\partial \chi_\beta} \; . \tag{15}$$

In general, the bracket in Eq. (15) does no longer satisfy the Jacobi relation

$$\mathcal{J} = \{\!\!\{a, \{\!\!\{b, c\}\!\!\}\}\!\!\} + \{\!\!\{c\{\!\!\{a, b\}\!\!\}\}\!\!\} + \{\!\!\{b, \{\!\!\{c, a\}\!\!\}\}\!\!\} \neq 0 \; . \tag{16}$$

Thus, non-Hamiltonian equations of motion can be written as

$$\frac{\partial \chi}{\partial t} = -\frac{i}{\hbar} \{\!\!\{\chi, h(\chi)\}\!\!\} \; . \tag{17}$$

If one defines the non-Hamiltonian probability current $J^{nH}$ as

$$J^{nH} = \frac{i}{\hbar} \begin{bmatrix} \mathcal{B}_{12}((f(r);\chi)h|\psi\rangle \\ \\ \langle\psi|h\mathcal{B}_{21}(f(r);\chi) \end{bmatrix} \; , \tag{18}$$

then the non-Hamiltonian continuity equation can be written as

$$\frac{\partial \rho}{\partial t} = -\frac{\partial}{\partial \chi} \cdot J^{nh} - \langle (\partial \mathcal{B}_{12}/\partial \chi_1 | h | \chi_1 \rangle - \langle \chi_2 | h | (\partial \mathcal{B}_{21}/\partial \chi_2 \rangle \; . \tag{19}$$

In principle, the non-Hamiltonian theory, specified by Eqs. (15), (16), (17), (18) and (19), can be used to address the problem of nonlinear correction to quantum mechanics following Refs. [1]. This will not be done here. Instead, the non-Hamiltonian structures will be analyzed in detail to see if they could be used to devise new calculation schemes for quantum mechanical systems. In the remaining of this paper, it will be assumed that the Hamiltonian function has a bilinear form as specified by Eq. (6). In such a case, one has

$$|(\partial h/\partial \chi_2)\rangle \;=\; \hat{H}|\psi\rangle \tag{20}$$

$$\langle(\partial h/\partial \chi_1)| \;=\; \langle\psi|\hat{H} \; , \tag{21}$$

so that the non-Hamiltonian equations of motion in (17) take the explicit form

$$\frac{\partial}{\partial t}|\psi\rangle \;=\; -\frac{i}{\hbar}\mathcal{B}_{12}\hat{H}|\psi\rangle \tag{22}$$

$$\frac{\partial}{\partial t}\langle\psi| \;=\; -\frac{i}{\hbar}\langle\psi|\hat{H}\mathcal{B}_{21} \; . \tag{23}$$

Equations (22-23) lead to the following time-dependent wave fields

$$|\psi(t)\rangle \;=\; \exp\left[-\frac{it}{\hbar}\mathcal{B}_{12}\hat{H}\right]|\psi\rangle \tag{24}$$

$$\langle\psi(t)| \;=\; \langle\psi|\exp\left[\frac{it}{\hbar}\hat{H}\mathcal{B}_{12}\right] \; , \tag{25}$$

where $\mathcal{B}_{12} = -\mathcal{B}_{21}$ has been used. Thus, the time dependence of average values in the Schrödinger picture is given by

$$\begin{aligned} a(t) &= \langle\psi(t)|\hat{A}|\psi(t)\rangle \\ &= \langle\psi|e^{(it/\hbar)\hat{H}\mathcal{B}_{12}}\hat{A}e^{-(it/\hbar)\mathcal{B}_{12}\hat{H}}|\psi\rangle \; . \end{aligned} \tag{26}$$

At this point, one would like to see how the Heisenberg picture, of the above non-Hamiltonian wave mechanics, is defined. To this end, one can consider the following operator identity [16]

$$e^{\hat{Y}}\hat{X}e^{-\hat{Y}} = e^{[\hat{Y},\ldots]}\hat{X} \; , \tag{27}$$

where $[\hat{Y},\ldots]\hat{X} \equiv [\hat{Y},\hat{X}]$. The identity in Eq. (27) is trivial to apply when $\mathcal{B}_{12} = 1$. In such a case it gives the usual Heisenberg picture of quantum mechanics [16]. In the non-Hamiltonian Schrödinger picture given in Eq. (26), $\mathcal{B}_{12}$ may be, instead, a function of coordinates and a functional of the wave fields. However, if one introduces the non-Hamiltonian commutator $[\![\ldots,\ldots]\!]$ as

$$\begin{aligned} [\![\hat{A}, \hat{B}]\!] &= \begin{bmatrix} \hat{A} & \hat{B} \end{bmatrix} \cdot \boldsymbol{\mathcal{B}} \cdot \begin{bmatrix} \hat{A} \\ \hat{B} \end{bmatrix} \\ &= \hat{A}\mathcal{B}_{12}\hat{B} - \hat{B}\mathcal{B}_{12}\hat{A} \; , \end{aligned} \tag{28}$$

it is not difficult to find by means of series expansion of the exponential operator that

$$
\begin{aligned}
a(t) &= \langle\psi|e^{(it/\hbar)\hat{H}\mathcal{B}_{12}}\hat{A}e^{-(it/\hbar)\mathcal{B}_{12}\hat{H}}|\psi\rangle \\
&= \langle\psi|\exp\left\{(it/\hbar)\llbracket\hat{H},\ldots\rrbracket\right\}\hat{A}|\psi\rangle \ .
\end{aligned} \tag{29}
$$

Equation (29) defines non-Hamiltonian equations of motion in the Heisenberg picture as

$$
\frac{d\hat{A}}{dt} = \frac{i}{\hbar}\llbracket\hat{H},\hat{A}\rrbracket \ . \tag{30}
$$

Equations (30) coincide with the equations proposed in Ref. [11].

## IV. QUANTUM-CLASSICAL WAVE DYNAMICS

In Ref. [11] it was shown that the quantum-classical algebra, as introduced in Refs. [10], can be considered as a particular realization of non-Hamiltonian commutators. To this end, denote the classical $2N$-dimensional phase space point by $X=(R,P)$. Then consider quantum operators which depends on the phase space point $\hat{\eta}=\hat{\eta}(X)$ and introduce the operator $\Lambda$ which, when sandwiched between two arbitrary quantum-classical variables, provides the negative of the Poisson bracket

$$
\begin{aligned}
\{\hat{\eta},\hat{\xi}\}_P &= -\hat{\eta}\Lambda\hat{\xi} \\
&= \sum_{i,j=1}^{2N}\frac{\partial\hat{\eta}}{\partial X_i}\mathcal{B}^c_{ij}\frac{\partial\hat{\xi}}{\partial X_j} \ .
\end{aligned} \tag{31}
$$

One can introduce an antisymmetric matrix operator

$$
\boldsymbol{\mathcal{D}} = \left[\begin{array}{cc} 0 & 1+\frac{\hbar}{2i}\Lambda \\ -1-\frac{\hbar}{2i}\Lambda & 0 \end{array}\right] \ , \tag{32}
$$

and by means of this define a quantum-classical commutator $\oint \ldots,\ldots \oint$ as

$$
\begin{aligned}
\oint \hat{\eta},\hat{\xi} \oint &= \frac{i}{\hbar}\left[\begin{array}{cc}\hat{\eta} & \hat{\xi}\end{array}\right]\cdot\boldsymbol{\mathcal{D}}\cdot\left[\begin{array}{c}\hat{\eta}\\ \hat{\xi}\end{array}\right] \\
&= \frac{i}{\hbar}[\hat{\eta},\hat{\xi}] - \frac{1}{2}\{\hat{\eta},\hat{\xi}\}_P + \frac{1}{2}\{\hat{\xi},\hat{\eta}\}_P \ ,
\end{aligned} \tag{33}
$$

which, as it can be seen from the last equality in the right hand side of Eq. (33), is exactly the quantum-classical bracket introduced in Refs. [10].

Given a quantum-classical Hamiltonian $\hat{H}_{qc} = \hat{H}_{qc}(X)$, time evolution in the class of quantum-classical theories of Refs. [10] has been proposed so far exclusively in the Heisenberg picture. In this scheme of motion operators evolve according to

$$
\begin{aligned}
\hat{\eta}(X,t) &= \exp\left\{t\oint\hat{H}_{qc},\ldots\oint\right\}\hat{\eta}(X) \\
&= \exp\{it\mathcal{L}\}\,\hat{\eta}(X) \ ,
\end{aligned} \tag{34}
$$

where the last equality defines the quantum-classical Liouville operator. Quantum-classical averages are calculated in this scheme of motion as

$$
\begin{aligned}
\langle\hat{\eta}\rangle(t) &= Tr'\int dX\hat{\rho}(X)\hat{\eta}(X,t) \\
&= Tr'\int dX\hat{\rho}(X,t)\hat{\eta}(X) \ ,
\end{aligned} \tag{35}
$$

where $\hat{\rho}(X)$ is the quantum-classical density matrix and $\hat{\rho}(X,t)=\exp\{-it\mathcal{L}\}\,\hat{\rho}(X)$.

Either evolving the dynamical variables or the density matrix, one is still within a Heisenberg picture, i.e. a form of generalized quantum-classical matrix mechanics. This theory has interesting formal features and certain number of numerical approaches have been proposed to integrate the dynamics and calculate correlation functions. However, the algorithms have been limited so far to short-time dynamics due mainly to statistical uncertainties growing with time. With this in mind, it would be interesting to see which features a quantum-classical theory would posses a scheme of motion where quantum-classical wave fields, instead of operators, are advanced in time. In order to obtain such a scheme, which must start from Eq. (34), one must derive an operator identity analogous to that in Eq. (27). Noting that

$$
\begin{aligned}
\exp\{it\mathcal{L}\}\hat{\eta} &= \exp\left\{t\oint\hat{H}_{qc},\ldots\oint\right\}\hat{\eta} \\
&= \exp\left\{t\left[\overrightarrow{\mathcal{H}}\times(\ldots)-(\ldots)\times\overleftarrow{\mathcal{H}}\right]\right\}\hat{\eta} \ ,
\end{aligned} \tag{36}
$$

such an identity can indeed be derived and it is

$$
\exp\left\{t\oint\hat{H}_{qc},\ldots\oint\right\}\hat{\eta} = \exp\left\{t\overrightarrow{\mathcal{H}}\right\}\hat{\eta}\exp\left\{-t\overleftarrow{\mathcal{H}}\right\} \ , \tag{37}
$$

where, following Ref. [13], the two operators

$$
\overrightarrow{\mathcal{H}} = \frac{i}{\hbar}\hat{H}_{qc} - \frac{1}{2}\sum_{i,j=1}^{2N}\frac{\partial\hat{H}_{qc}}{\partial X_i}\mathcal{B}^c_{ij}\frac{\overrightarrow{\partial}}{\partial X_j} \tag{38}
$$

$$
\overleftarrow{\mathcal{H}} = \frac{i}{\hbar}\hat{H}_{qc} - \frac{1}{2}\sum_{i,j=1}^{2N}\frac{\overleftarrow{\partial}}{\partial X_i}\mathcal{B}^c_{ij}\frac{\partial\hat{H}_{qc}}{\partial X_j} \tag{39}
$$

have been introduced.

In order to introduce a wave picture for quantum-classical mechanics one can introduce quantum-classical wave fields, $|\psi(X)\rangle$ and $\langle\psi(X)|$, and make the following *ansatz* [18] for the density matrix

$$
\hat{\rho}(X) = \sum_i w_i|\psi^i(X)\rangle\langle\psi^i(X)| \ , \tag{40}
$$

where one has assumed that, because of thermal disorder, there can be many states $|\psi^i(X)\rangle$ $(i=1,\ldots,l)$ compatible with the macroscopic value of the measured observables [19]. Using the *ansatz* of Eq. (40) in Eq. (35), quantum classical averages can be written in this wave picture as

$$
\begin{aligned}
\langle\hat{\eta}\rangle(t) &= \int dX \sum_i w_i \langle\psi^i(X)|e^{it\mathcal{L}}\hat{\eta}|\psi^i(X)\rangle \\
&= \int dX \sum_i w_i \langle\psi^i(X)|e^{t\overrightarrow{\mathcal{H}}}\hat{\eta}e^{-t\overleftarrow{\mathcal{H}}}|\psi^i(X)\rangle \, .
\end{aligned}
\tag{41}
$$

Recalling the definitions in Eq. (38) and (39), and exploiting the antisymmetry of $\boldsymbol{\mathcal{B}}^c$, one can define the time dependence of the wave fields as

$$
|\psi^i(X,t)\rangle = \exp\left[-\frac{it}{\hbar}\hat{H}_{qc} - \frac{t}{2}\sum_{k,j=1}^{2N}\frac{\partial \hat{H}_{qc}}{\partial X_j}\mathcal{B}^c_{jk}\frac{\partial\ldots}{\partial X_k}\right]|\psi^i(X)\rangle
\tag{42}
$$

$$
\langle\psi^i(X,t)| = \langle\psi^i(X)|\exp\left[\frac{it}{\hbar}\hat{H}_{qc} + \frac{t}{2}\sum_{k,j=1}^{2N}\frac{\partial\ldots}{\partial X_j}\mathcal{B}^c_{jk}\frac{\partial \hat{H}_{qc}}{\partial X_k}\right] \, .
\tag{43}
$$

These lead to the two following wave equations

$$
\begin{aligned}
\frac{\partial}{\partial t}|\psi^i(X,t)\rangle &= -\frac{i}{\hbar}\hat{H}_{qc}|\psi^i(X,t)\rangle \\
&- \frac{1}{2}\sum_{k,j=1}^{2N}\frac{\partial \hat{H}_{qc}}{\partial X_j}\mathcal{B}^c_{jk}\frac{\partial|\psi^i(X,t)\rangle}{\partial X_k}
\end{aligned}
\tag{44}
$$

$$
\begin{aligned}
\langle\psi^i(X,t)|\frac{\partial}{\partial t} &= +\langle\psi^i(X,t)|\hat{H}_{qc}\frac{i}{\hbar} \\
&+ \frac{1}{2}\sum_{k,j=1}^{2N}\frac{\partial\langle\psi^i(X,t)|}{\partial X_j}\mathcal{B}^c_{jk}\frac{\partial \hat{H}_{qc}}{\partial X_k}
\end{aligned}
\tag{45}
$$

These equations can be simplified if one assumes that $\hat{H}_{qc} = (P^2/2M) + \hat{h}(R)$, where the first term gives the kinetic energy of the classical degrees of freedom while $\hat{h}(R)$ is the Hamiltonian operator describing kinetic and potential quantum energies and the coupling of these with the classical coordinates $R$. In such a case, the quantum-classical wave equations of motion can be written as

$$
\begin{aligned}
\frac{\partial}{\partial t}|\psi^i(X,t)\rangle &= -\frac{i}{\hbar}\hat{H}_{qc}|\psi^i(X,t)\rangle - \frac{1}{2}\frac{\partial\hat{H}_{qc}}{\partial R}\frac{\partial|\psi^i(X,t)\rangle}{\partial P} \\
&+ \frac{1}{2}\frac{P}{M}\frac{\partial|\psi^i(X,t)\rangle}{\partial R}
\end{aligned}
\tag{46}
$$

$$
\begin{aligned}
\langle\psi^i(X,t)|\frac{\partial}{\partial t} &= \langle\psi^i(X,t)|\hat{H}_{qc}\frac{i}{\hbar} + \frac{1}{2}\frac{\partial\langle\psi^i(X,t)|}{\partial R}\frac{P}{M} \\
&- \frac{1}{2}\frac{\partial\langle\psi^i(X,t)|}{\partial P}\frac{\partial\hat{H}_{qc}}{\partial R} \, .
\end{aligned}
\tag{47}
$$

Now define the operator

$$
\begin{aligned}
\overrightarrow{S} &= -\frac{i}{\hbar}\left[\hat{H}_{qc} + \frac{\hbar}{2i}\left(\frac{\partial\hat{H}_{qc}}{\partial R}\frac{\overrightarrow{\partial}}{\partial P} - \frac{P}{M}\frac{\overrightarrow{\partial}}{\partial R}\right)\right] \\
&= -\frac{i}{\hbar}\left[\hat{H}_{qc} + \frac{\hbar}{2i}\{\hat{H}_{qc},\ldots\}_P\right] \, ,
\end{aligned}
\tag{48}
$$

$$
\begin{aligned}
\overleftarrow{S} &= \frac{i}{\hbar}\left[\hat{H}_{qc} + \frac{\hbar}{2i}\left(\frac{\overleftarrow{\partial}}{\partial R}\frac{P}{M} - \frac{\overleftarrow{\partial}}{\partial R}\frac{\partial\hat{H}_{qc}}{\partial R}\right)\right] \\
&= \frac{i}{\hbar}\left[\hat{H}_{qc} + \frac{\hbar}{2i}\{\ldots,\hat{H}_{qc}\}_P\right] \, .
\end{aligned}
\tag{49}
$$

It is not difficult to see that

$$
\left[\exp\left(t\overrightarrow{S}\right)\right]^\dagger = \exp\left(-t\overleftarrow{S}\right) \, ,
\tag{50}
$$

so that the unitary property of quantum-classical dynamics is also retained in the above wave picture. It is also worth noting that by defining a quantum-classical Hamiltonian functions, analogous to the observables defined by Weinberg [1], as

$$
\begin{aligned}
h^i_{qc}(X) &= \langle\psi^i(X)|\hat{H}_{qc}|\psi^i(X)\rangle \\
&+ \frac{\hbar}{2i}\Big(\langle\psi^i(X)|\{\hat{H}_{qc},|\psi^i(X)\rangle\}_P \\
&+ \{\langle\psi^i(X)|,\hat{H}_{qc}\}_P|\psi^i(X)\rangle\Big) \, ,
\end{aligned}
\tag{51}
$$

so that

$$
\frac{\partial h^i_{qc}(X)}{\partial\langle\psi^i(X)|} = \hat{H}_{qc}|\psi^i(X)\rangle + \frac{\hbar}{2i}\{\hat{H}_{qc},|\psi^i(X)\rangle\}_P \, ,
\tag{52}
$$

$$
\frac{\partial h^i_{qc}(X)}{\partial|\psi^i(X)\rangle} = \langle\psi^i(X)|\hat{H}_{qc} + \frac{\hbar}{2i}\{\langle\psi^i(X)|,\hat{H}_{qc}\}_P \, .
\tag{53}
$$

Then, equations of motion can be written as

$$
\frac{\partial|\psi^i(X)\rangle}{\partial t} = -\frac{i}{\hbar}\frac{\partial h^i_{qc}(X)}{\partial\langle\psi^i(X)|} \, ,
\tag{54}
$$

$$
\frac{\partial\langle\psi^i(X)|}{\partial t} = \frac{i}{\hbar}\frac{\partial h^i_{qc}(X)}{\partial|\psi^i(X)\rangle} \, .
\tag{55}
$$

By using Weinberg's bracket as given in Eq. (4), but which must be defined, this time, in terms of the wave fields $\langle\psi^i(X)|$ and $|\psi^i(X)\rangle$, Eqs (54) and (55), can be written in compact form as

$$
\frac{\partial\chi^i(X)}{\partial t} = -\frac{i}{\hbar}\{\hat{H}_{qc},\chi^i(X)\} \, ,
\tag{56}
$$

where

$$
\chi^i(X) = \begin{bmatrix} |\psi^i(X)\rangle \\ \langle\psi^i(X)| \end{bmatrix} \, .
\tag{57}
$$

Equations (46) and (47) or their compact "Weinberg-like" form in Eq. (57), provide the searched wave picture of quantum-classical dynamics. In this scheme of motion, averages are calculated according to

$$
\langle\hat{\eta}\rangle(t) = \int dX \sum_i w_i\langle\psi^i(X,t)|\hat{\eta}(X)|\psi^i(X,t)\rangle \, ,
\tag{58}
$$

where one must advance in time the wave fields, keep constant the microscopic quantum classical operator corresponding to the quantity one wants to calculate, and know or calculate the weights $w_i$ which takes into account the thermal disorder.

Future works will be devoted to devise numerical integration schemes for Eqs. (46) and (47) and to calculate averages according to Eq. (58).

## V. CONCLUSIONS

In this paper the symplectic structure of the formalism, Weinberg proposed originally in order to describe nonlinear effects in quantum mechanics, has been unveiled. By generalizing the symplectic matrix entering the definition of the Poisson bracket, which was used by Weinberg, one could define non-Hamiltonian brackets which no longer satisfy the Jacobi relation. Therefore, a non-Hamiltonian theory of quantum mechanics is obtained. Within this scheme, nonlinear effects can be introduced formally by exploiting the general antisymmetric matrix entering the definition of the non-Hamiltonian bracket. Thus, in contrast to Weinberg's approach, it is no longer necessary to abandon the usual bilinear definition of the Hamiltonian function. It remains to be determined if and which advantages this non-Hamiltonian formalism provides when treating nonlinear effects. This issue will be treated in future works. Here, by exploiting the general connection between wave and matrix mechanics, non-Hamiltonian wave mechanics has been recasted to be expressed as a matrix mechanics by means of the non-Hamiltonian commutator introduced recently by this author. The connection between "Heisenberg-like" quantum-classical mechanics, expressed by means of time evolving quantum-classical operators, and the "Schrödinger-like" formalism, according to which quantum-classical wave functions are evolved in time, can be considered as a first step toward a deeper understanding of the differences between quantum-classical evolution of operators and schemes where wave functions are propagated in time while classical degrees of freedom follows surface-hopping trajectories on single quantum states.

As it has been shown in a previous paper by this author, quantum-classical mechanics is a particular realization of non-Hamiltonian quantum mechanics. In other words, one could define a non-Hamiltonian quantum commutator which coincides with the quantum-classical bracket other authors proposed in the literature. In this paper, by deriving a connection between matrix and wave mechanics in the quantum-classical case, it has been obtained a scheme of quantum-classical motion where wave fields are advanced in time. There is hope that this wave formulation of quantum-classical mechanics could provide hints to solve the difficult problem of long-time numerical integration of quantum-classical (and quantum) dynamics. Future works will be devoted specifically to the investigation of numerical algorithms for simulating the quantum-classical dynamics of wave functions and for calculating averages within this approach.


### Acknowledgment

This author is grateful to Professor Raymond Kapral for suggesting him the possibility of mapping "Heisenberg-like" quantum-classical dynamics to a wave scheme of motion motion.


## APPENDIX A: AN IDENTITY FOR QUANTUM-CLASSICAL OPERATORS

Consider the identity in Eq. (37). It can be proved by some algebra considering that the quantum-classical commutator can be written as

$$\llbracket \hat{H}_{qc}, \hat{\eta} \rrbracket = \overrightarrow{\mathcal{H}}\hat{\eta} - \hat{\eta}\overleftarrow{\mathcal{H}} \; . \tag{A1}$$

Then by Taylor expanding the quantum-classical propagator of the "Heisenberg-like" scheme of motion, one obtains

$$\begin{aligned} \exp\left\{\llbracket \hat{H}_{qc}, \ldots \rrbracket\right\}\hat{\eta} &= \approx \left\{1 + t\llbracket \hat{H}_{qc}, \ldots \rrbracket \right. \\ &+ \left. \frac{t^2}{2}\llbracket \hat{H}_{qc}, \llbracket \hat{H}_{qc}, \ldots \rrbracket \rrbracket + \ldots \right\}\hat{\eta} \\ &= \hat{\eta} + t\left(\overrightarrow{\mathcal{H}}\hat{\eta} - \hat{\eta}\overleftarrow{\mathcal{H}}\right) \\ &+ \frac{t^2}{2}\left(\overrightarrow{\mathcal{H}}\overrightarrow{\mathcal{H}}\hat{\eta} - 2\overrightarrow{\mathcal{H}}\hat{\eta}\overleftarrow{\mathcal{H}} + \hat{\eta}\overleftarrow{\mathcal{H}}\overleftarrow{\mathcal{H}}\right) + \ldots \end{aligned} \tag{A2}$$

One can also Taylor expand the operator in the right hand side of Eq. (37)

$$\begin{aligned} e^{t\overrightarrow{\mathcal{H}}}\hat{\eta}e^{-t\overleftarrow{\mathcal{H}}} &= \left(1 + t\overrightarrow{\mathcal{H}} + \frac{t^2}{2}\overrightarrow{\mathcal{H}}\overrightarrow{\mathcal{H}} + \ldots\right)\hat{\eta} \\ &\times \left(1 - t\overleftarrow{\mathcal{H}} + \frac{t^2}{2}\overleftarrow{\mathcal{H}}\overleftarrow{\mathcal{H}} - \ldots\right) \\ &= \hat{\eta} + t\left(\overrightarrow{\mathcal{H}}\hat{\eta} - \hat{\eta}\overleftarrow{\mathcal{H}}\right) \\ &+ \frac{t^2}{2}\left(\overrightarrow{\mathcal{H}}\overrightarrow{\mathcal{H}}\hat{\eta} - 2\overrightarrow{\mathcal{H}}\hat{\eta}\overleftarrow{\mathcal{H}} + \hat{\eta}\overleftarrow{\mathcal{H}}\overleftarrow{\mathcal{H}}\right) + \ldots \end{aligned} \tag{A3}$$

One realizes that the right hand sides of Eqs. (A2) and (A3) coincides. This has been done explicitly up to second order in $t$. However, with additional algebra it can be proved for every term in the expansion of the exponential operators.

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