Mixing Quantum and Classical Mechanics

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Abstract

Using a group theoretical approach we derive an equation of motion for a mixed quantum-classical system. The quantum-classical bracket entering the equation preserves the Lie algebra structure of quantum and classical mechanics: The bracket is antisymmetric and satisfies the Jacobi identity, and, therefore, leads to a natural description of interaction between quantum and classical degrees of freedom. We apply the formalism to coupled quantum and classical oscillators and show how various approximations, such as the mean-field and the multiconfiguration mean-field approaches, can be obtained from the quantum-classical equation of motion.

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1 Introduction

Many phenomena in nature are described by quantum mechanics at a fundamental level and with high precision. Yet, there exist numerous situations where mixed quantum-classical models are needed. In some cases the phenomena are too complex to allow for a fully quantum approach, in others a consistent quantum theory is lacking. Classical mechanics often provides a more suggestive description and a clearer picture of physical events. Applications of various quantum-classical approaches range from biochemical and condensed matter chemical reactions, where the large dimensionality of the systems of interest requires approximations, to the evolution of the universe and cosmology, where no theory of quantum gravity has been established.

The issue of treating quantum and classical degrees of freedom within the same formalism was recently discussed in a number of publications [1, 2, 3]. The interest was spurred by the cosmological problem of defining the backreaction of quantum matter fields on the classical space-time background, where classical variables should be independently correlated with each individual quantum state. The traditional approach fails to satisfy the last requirement. (For a fully quantum approach to cosmology see reference [4].) Somewhat earlier a similar situation was encountered in chemical physics, where quantum-classical trajectory methods were employed to model gas phase scattering phenomena and chemical dynamics in liquids [5, 6, 7, 8, 9, 10]. It was noticed in these studies that asymptotically distinct quantum evolutions should correlate with different classical trajectories.

The first relationship between quantum and classical variables is due to Ehrenfest [11] who showed that the equation of motion for the average values of quantum observables coincides with the corresponding classical expression. (Surprisingly, the first mathematically rigorous treatment on the subject was not carried out until 1974, see reference [12].) Ehrenfest's result leads to the mean-field approach, where classical dynamics is coupled to the evolution of the expectation values of quantum variables [13, 14, 15, 16]. The mean-field equations of motion possess all of the properties of the purely classical equations and are exact as far as the mean values of quantum operators are concerned. However, an expectation value does not provide information of the outcome of an individual process. The mean-field approach gives a satisfactory description of the classical subsystem as long as changes within the quantum part are fast compared to the characteristic classical time-scale. If classical trajectories depend strongly on a particular realization of the quantum evolution, the mean field approximation is inadequate. The problem can be corrected, for instance by introduction of stochastic quantum hops between preferred basis states with probabilities determined by the usual quantum-mechanical rules [17, 18, 19].

Similarity between the algebraic structures underlying quantum and classical mechanics provides a consistent way of improving upon the mean-field approximation, as explored in references [2, 3, 6]. In those studies the aim was to derive a quantum-classical bracket that reduces to the quantum commutator and the Poisson bracket in the purely quantum and classical cases. In addition to the reduction property the bracket should satisfy other criteria so as to give physically meaningful pictures of quantum-classical evolutions. In particular, an antisymmetric bracket conserves the total energy and a bracket satisfying the Jacobi identity ensures that the Heisenberg uncertainty principle is not violated.

Recently, one of us (VVK) proposed [20] a natural mathematical construction, which we name p-mechanics, enveloping classical and quantum mechanics. Formulated within the framework of operator algebras, the p-mechanical equation of motion reduces to the appropriate quantum or classical equations under suitable representations of the algebra of observables. In this paper we extend the ideas of p-mechanics to incorporate mixed quantum-classical descriptions. In particular, we derive the quantum-classical bracket and explicitly show that it satisfies the properties common to quantum and classical mechanics. Using the technique described it is possible to construct families of mixed quantum-classical approaches, each having a specific set of properties.

The format of this paper is as follows: In Section 2 we summarize p-mechanics and introduce the essential mathematical definitions. In Section 3 we construct the simplest

p-mechanical model that adopts two distinct sets of variables associated with quantum and classical degrees of freedom. By taking the appropriate representation we derive the quantum-classical bracket and show that it is antisymmetric and obeys the Jacobi identity, that is, it possesses the two major properties shared by the quantum and classical brackets. In Section 4 we work out the case of coupled classical and quantum harmonic oscillators. Finally, in Section 5 we discuss how various approximations to the general quantum-classical description can be obtained, including the mean-field and the multiconfiguration mean-field approaches.

2 P-mechanics

2.1 The Elements of P-mechanics

We recall the constructions from references [20, 21] together with appropriate modifications.

Definition 1 An operator algebra $\mathfrak{P}$ gives a *p-mechanical description* [20] of a system if the following conditions hold.

1.1. The set $\widehat{\mathfrak{P}}$ of all irreducible representations π_h of $\mathfrak{P}$ is a disjoint union of subsets $\widehat{\mathfrak{P}} = \sqcup_{p\in P}\widehat{\mathfrak{P}}_p$ parameterized by the elements of a set P. The elements of the set P are associated with different values for the Planck constant. We refer to this set as the *set of Planck constants*. If for p_0 the set $\widehat{\mathfrak{P}}_{p_0}$ consists of only commutative (and, therefore, one-dimensional) representations, then $\widehat{\mathfrak{P}}_{p_0}$ gives a *classical* description. If $\widehat{\mathfrak{P}}_{p_0} = \{\pi_{p_0}\}$ consists of a single non-commutative representation π_{p_0}, then $\widehat{\mathfrak{P}}_{p_0}$ gives a purely *quantum* model. Sets $\widehat{\mathfrak{P}}_p$ of other types provide *mixed* (quantum-classical) descriptions.

1.2. Let $\widehat{\mathfrak{P}}$ be equipped with a natural operator topology (for example, it may be the Jacobson topology [22] or the *-bundle topology [23, 24]). Then P has a natural *factor topology* induced by the partition $\widehat{\mathfrak{P}} = \sqcup_{p\in P}$.

1.3. (Dynamics) The algebra $\mathfrak{P}$ is equipped with the one-parameter semigroup of transformations $G(t) : \mathfrak{P} \to \mathfrak{P}$, $t \in \mathbb{R}^+$. All sets $\widehat{\mathfrak{P}}_p$, $p \in P$ are *preserved* by $G(t)$. Namely, for any $\pi \in \widehat{\mathfrak{P}}_p$ all new representations $\pi_t = \pi \circ G(t)$ again belong to $\widehat{\mathfrak{P}}_p$.

1.4. (The Correspondence Principle) Let $S : p \mapsto S(p) \in \mathfrak{P}_p$ be an operator-valued section continuous in the *-bundle topology [23, 24] over P. Then for any t, i.e., at any moment of time the image $S_t(p) = G(t)S(p)$ is also a section due to statement 1.3. In the *-bundle topology the sections $S_t(p)$ are *continuous for all* t.

Having listed these quite natural conditions, we do not yet know how to construct p-mechanics. Next, we describe an important particular case of *group quantization* [21]. All components of p-mechanics (operator algebra, partition of representations, topology) readily arise there.

Construction 2 *Group quantization* consists of the following steps.

2.1. Let $\Omega = \{x_j\}, 1 \leq j \leq N$ be a set of physical variables defining the state of a classical system. Classical observables are real-valued functions on the states.

The best known and the most important case is the set $\{x_j = q_j, x_{j+n} = p_j\},\ 1 \leq j \leq n, N = 2n$ of coordinates and momenta of classical particles forming an n degree of freedom system. The observables are real valued functions on $\mathbb{R}^{2n}$. We will use this example throughout this Section.

2.2. We complete the set Ω with additional variables $x_j, N < j \leq \bar{N}$, such that the new set $\bar{\Omega}$ forms the smallest algebra, which contains Ω and is closed under the Poisson bracket

$$\{x_i, x_j\} \in \bar{\Omega}, \quad \text{for all } x_i, x_j \in \bar{\Omega}.$$

In the above example we add the unit function $x_{2n+1} = 1$. The complete set contains $\bar{N} = 2n + 1$ elements satisfying the famous relations

$$\{x_j, x_{j+n}\} = -\{x_{j+n}, x_j\} = x_{2n+1}. \tag{1}$$

All other Poisson brackets are zero.

2.3. We form an $\bar{N}$-dimensional Lie algebra $\mathfrak{p}$ with the frame $\{\widehat{x}_j\}$, $1 \leq j \leq \bar{N}$ defined by the formal mapping $\widehat{}: x_j \mapsto \widehat{x}_j$. The commutators of the frame vectors are formally defined by the formula

$$[\widehat{x}_i, \widehat{x}_j] = \widehat{\{x_i, x_j\}}. \tag{2}$$

We extend the commutator onto the whole algebra by linearity.

For our example, $\mathfrak{p}$ is the Lie algebra corresponding to the Heisenberg group (see the next Subsection for details).

2.4. We introduce the algebra $\mathfrak{P}$ of convolutions induced by $\mathfrak{p}$. The convolution operators are *observables* in the group quantization, and by analogy with the classical case they can be treated as functions of $\widehat{x}_j$. Particular representations of the convolution algebra in spaces $\mathbb{L}^2(S)$ give different descriptions of a physical system. The family of all one-dimensional representations of $\mathfrak{P}$ corresponds to *classical* mechanics; various noncommutative representations lead to *quantum* and *quantum-classical* descriptions with different *Planck constants.*

For our example the following possibilities exist.

(a) $S = \mathbb{R}^n$, $\widehat{x}_j = X_j = M_{q_j}$, $\widehat{x}_{j+n} = -i\hbar\partial/\partial q_j$, the convolutions are represented by pseudo-differential operators (PDO), and we obtain the *Dirac-Heisenberg-Schrödinger-Weyl quantization* by PDO.

(b) $S = \mathbb{R}^{2n}$, $\widehat{x}_j = X_j = M_{q_j}$, $\widehat{x}_{j+n} = M_{p_j}$, the convolutions are represented by (operators of multiplication by) functions, and we obtain the classical description that we started from.

It is an empirical observation that *the steps above lead to a nilpotent Lie group, with the dual $\widehat{Z}$ of the center Z of the group interpreted as the set of Planck constants.* Now we illustrate this fact by a well-known example of quantization, and later in Section 3 by constructing a quantum-classical model.

2.2 The Heisenberg Group Generates Quantum and Classic Mechanics

In the previous Subsection we claimed that the nth order Heisenberg group $\mathbb{H}^n$ describes a set of quantum particles that constitute an n-degree of freedom system. Here we show how this description is achieved.

$\mathbb{H}^n$ is generated by the n-dimensional translation and multiplication operators $e^{ip\cdot D}$, $e^{iq\cdot X}$, $p, q \in \mathbb{R}^n$ satisfying the Weyl commutator relations

$$e^{2\pi ip\cdot D}e^{2\pi iq\cdot X} = e^{2\pi ip\cdot q}e^{2\pi iq\cdot X}e^{2\pi ip\cdot D}. \tag{3}$$

An element of the Heisenberg group $g \in \mathbb{H}^n$ is defined by $2n+1$ real numbers (p, q, s), $p, q \in \mathbb{R}^n$, $s \in \mathbb{R}$. The composition of two elements g and g' is given by

$$(p, q, s)(p', q', s') = (p + p', q + q', s + s' + \frac{1}{2}(pq' - p'q)).$$

D_j, X_j, and I form a $2n+1$ dimensional basis of the Heisenberg algebra $\mathfrak{h}^n$ with a one-dimensional center $\mathbb{Z} = \{sI; s \in \mathbb{R}\}$. Since all second and higher order commutators of the basis elements vanish, $\mathbb{H}^n$ and $\mathfrak{h}^n$ are step two nilpotent Lie group and algebra respectively.

The unitary irreducible representations of the Heisenberg group are classified by the Stone-von Neumann theorem [25]. They are parameterized by a real number h, the character of the one-dimensional center $\mathbb{Z}$. A non-zero h gives non-commutative unitary representations acting on the Hilbert space $L^2(\mathbb{R}^n)$

$$\rho_{h\neq 0}(p, q, s) = e^{2\pi i(p\cdot hD+q\cdot X+s\cdot hI)}. \tag{4}$$

The n components of X and hD are the usual quantum mechanical position X_j (multiplication by x_j) and momentum hD_j ($-i\hbar$ times differentiation with respect to x_j) operators characterized by the Heisenberg commutator relation

$$[hD_j, X_k] = -ih\delta_{jk}I. \tag{5}$$

In the limit of zero h the center $\mathbb{Z}$ of the Heisenberg group vanishes, and $\mathbb{H}^n$ becomes isomorphic to $\mathbb{R}^{2n}$. The irreducible representations of the latter are homomorphisms from $\mathbb{R}^{2n}$ into the circle group acting on $\mathbb{C}$

$$\rho_{h=0}(p,q) = e^{2\pi i(pk+qx)}. \tag{6}$$

The dual $\widehat{\mathbb{H}}^n$ as a set is equal to $\{\mathbb{R}\setminus 0\}\cup\mathbb{R}^{2n}$ (see Figure 1). It has the natural topology coinciding on $\{\mathbb{R}\setminus 0\}$ with the Euclidean topology. Any sequence of representations $\{\rho_{h_j}\}$, $h_j \to 0$, $h_j \neq 0$ is dense in whole $\mathbb{R}^{2n}$. The last property is fundamental for the *correspondence principle.*

The unitary representations of $\mathbb{H}^n$ can be extended to the convolution algebra $L^1(\mathbb{H}^n)$. Namely, if $A \in L^1(\mathbb{H}^n)$, then it defines a convolution on the Heisenberg group

$$A\cdot b(g) = \int_{\mathbb{H}^n} A(g')b(g\star g')dg'.$$

The representation ρ_h maps the convolution to the operator

$$\begin{aligned}\rho_h(A) &= \int_{\mathbb{H}^n} A(g)\rho_h(g)dg \\ &= \int\int\int A(p,q,s)\rho_h(p,q,s)dpdqds.\end{aligned} \tag{7}$$

The p-mechanical equation of motion (see [20] for details) for an element $A(g)$ ($g \equiv \{p,q\}$) of the convolution algebra is defined by

$$\frac{\partial A(g)}{\partial t} = 2\pi i[H,A](g) \tag{8}$$

with

$$[H,A](g) = \int_{\mathbb{H}^n} [H(g')A(g'*g) - A(g')H(g'*g)]dg',$$

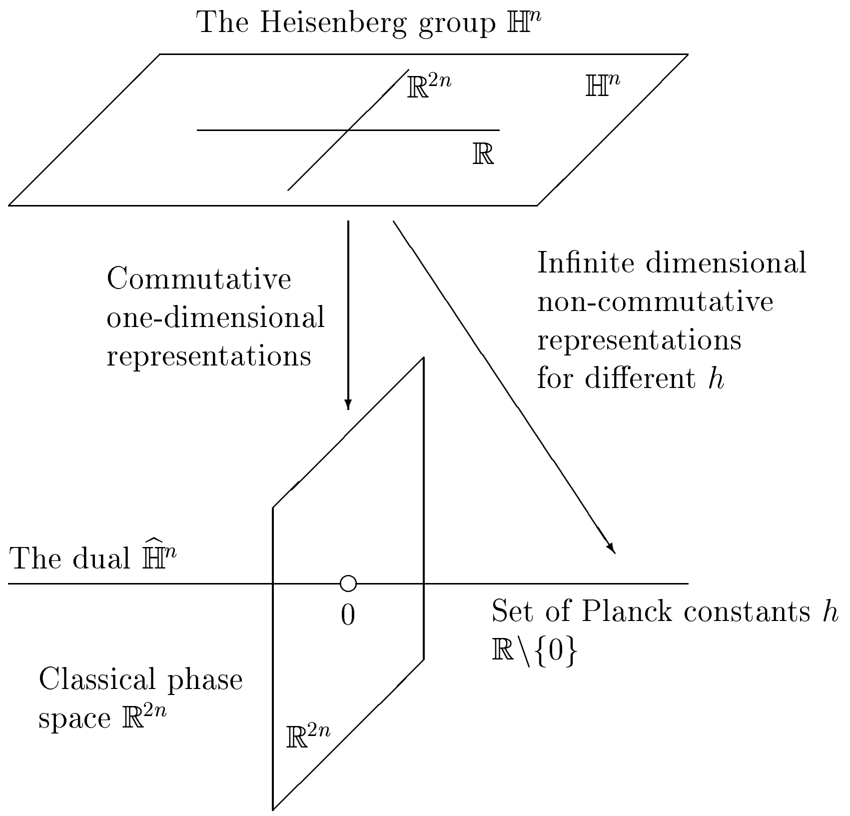

Figure 1: The Heisenberg group and its dual.

where $H(g)$ is the Hamiltonian. The non-commutative unitary representations of Eq. (4) reduce this equation to the Heisenberg equation of motion for operators acting on the Hilbert space $L^2(\mathbb{R}^n)$. Under the commutative representations of Eq. (6) the p-mechanical equation of motion becomes the Hamilton equation for functions on the phase space $\mathbb{R}^{2n}$.

We consider the last statement in more detail by means of the pseudo-differential calculus directly related to these group theoretical developments and the problem of quantization. The non-commutative unitary representations of the Heisenberg group allow one to define integral operators corresponding to functions on phase space. Given a function $\sigma(k, x)$ on

$\mathbb{R}^{2n}$ one obtains the operator $\sigma(D,X)$ on $L^2(\mathbb{R}^n)$ by the formula

$$\begin{aligned}\sigma(hD,X) &= \int_{\mathbb{H}^n} \mathcal{F}^{-1}[\sigma](g)\rho_{h\neq 0}(g)dg \\ &= \int\int \mathcal{F}^{-1}[\sigma](p,q)e^{2\pi i(p\cdot hD+q\cdot X)}dpdq, \end{aligned} \tag{9}$$

where $\mathcal{F}^{-1}[\bullet]$ denotes the inverse Fourier transform. The trivial integration over s has been carried out. The action of the operator $\sigma(D,X)$ on a function $f(x)\in L^2(\mathbb{R}^n)$ follows from the definition of hD and X [see Eq. (4) and the related paragraph], and is given by

$$\begin{aligned}\sigma(hD,X)f(x) &= \int\int \mathcal{F}^{-1}[\sigma](p,q)e^{\pi ihpq+2\pi iqx}f(x+hp)dpdq \\ &= h^{-n}\int\int \mathcal{F}^{-1}[\sigma](\frac{y-x}{h},q)e^{\pi iq(x+y)}f(y)dydq \\ &= h^{-n}\int\int \sigma(k,\frac{x+y}{2})e^{2\pi i(x-y)k/h}f(y)dydk \end{aligned} \tag{10}$$

or

$$\begin{aligned}\sigma(hD,X)f(x) &= \int K_\sigma(x,y)f(y)dy, \\ K_\sigma(x,y) &= h^{-n}\int \sigma(k,\frac{x+y}{2})e^{2\pi i(x-y)k/h}dk, \end{aligned} \tag{11}$$

where K_σ is the kernel of the integral operator $\sigma(hD,X)$. In the language of the pseudo-differential calculus the function $\sigma(k,x)$ is called the symbol of the operator $\sigma(hD,X)$. If instead of $\rho_{h\neq 0}$ one uses a commutative representation $\rho_{h=0}$, the transformation of Eq. (9) reduces to identity and we recover the *classical observable* $\sigma(k,x)$. Eqs. (9)–(11) are known as the Weyl correspondence principle.

The symbol $\sigma\sharp_h\tau$(k,x) of the product of two operators $\sigma\sharp_h\tau(hD,X)=\sigma(hD,X)\cdot\tau(hD,X)$ can be obtained by application of a non-commutative representation to the convolution on the Heisenberg group [see Eq. (7)] or directly from the Weyl rule. It is given in terms of the symbols of individual operators as

$$\sigma\sharp_h\tau(k,x) = \left(\frac{2}{h}\right)^{2n}\int\int\int\int \sigma(\zeta,u)\tau(\eta,v)e^{4\pi i[(x-u)(k-\eta)-(x-v)(k-\zeta)]/h}dudvd\eta d\zeta. \tag{12}$$

It follows from the discussion above that the non-commutative representations of the Heisenberg group transform the p-mechanical equation of motion (8) into the equation for operators on $L^2(\mathbb{R}^n)$

$$\frac{\partial}{\partial t}A(hD,X) \quad = \quad \frac{2\pi i}{h}[H,A]_{\sharp_h}(hD,X) \tag{13}$$

where $[H,A]_{\sharp_h} \equiv [H\sharp_h A - A\sharp_h H]$, the operation of taking the product of two symbols $\sharp_h$ is defined by Eq. (12), and the operators $A(hD,X)$ and $[H,A]_{\sharp_h}(hD,X)$ are recovered from their symbols $A(k,x)$ and $[H,A]_{\sharp_h}(k,x)$ by the application of the Weyl transform Eqs. (9)–(11). This is the quantum-mechanical law of motion in the Heisenberg form.

In order to obtain the corresponding classical expression it is useful to cast the product rule of Eq. (12) in the form of an asymptotic expansion in powers of h. The integration over η and ζ and the change of variables $(u-x)/h \to u$, $(v-x)/h \to v$ converts Eq. (12) to

$$\sigma\sharp_h\tau(k,x) \quad = \quad h^{-2n}\int\int \mathcal{F}_1^{-1}[\sigma](v,x+uh)\mathcal{F}_1[\tau](u,x+vh)e^{4\pi i(v-u)k}dudv,$$

where $\mathcal{F}_1$ and $\mathcal{F}_1^{-1}$ denote the Fourier transform and its inverse with respect to the first variable only. Expanding σ and τ in the second variable around x and applying the Fourier inversion formula to each term in the Taylor series we obtain

$$\begin{aligned}\sigma\sharp_h\tau(k,x) \quad &= \quad \sum_{\alpha+\beta\leq\gamma}\frac{(i\pi h)^{\alpha+\beta}(-1)^\alpha}{\alpha!\beta!}D_k^\beta D_x^\alpha\sigma(k,x)D_k^\alpha D_x^\beta\tau(k,x)+O(h^\gamma)\\ &= \quad \sum_{j=0}^{\gamma}\frac{(i\pi h)^j}{j!}[D_{k,\sigma}D_{x,\tau}-D_{k,\tau}D_{x,\sigma}]^j\sigma(k,x)\tau(k,x)+O(h^\gamma),\end{aligned} \tag{14}$$

where the second subscripts σ and τ of D indicate the symbol to be acted upon. The asymptotic expression for the symbol of the commutator of two operators follows from Eq. (14). The even order terms in the sum cancel out to produce

$$\begin{aligned}[\sigma\sharp_h\tau-\tau\sharp_h\sigma](k,x) \quad &= \quad 2i\sum_{j=0}^{\gamma}\frac{(-1)^j(\pi h)^{2j+1}}{(2j+1)!}[D_{k,\sigma}D_{x,\tau}-D_{k,\tau}D_{x,\sigma}]^{2j+1}\sigma(k,x)\tau(k,x)\\ &+ \quad O(h^{2\gamma+1}).\end{aligned} \tag{15}$$

The series expansion of the symbol of the commutator Eq. (15) allows to derive the Poisson bracket as the classical limit of the symbol of the Heisenberg commutator of two quantum operators

$$\lim_{h\to 0} \frac{2\pi i}{h}[\sigma\sharp_h\tau - \tau\sharp_h\sigma](k,x) \quad = \quad \{\sigma(k,x), \tau(k,x)\}. \tag{16}$$

Since the commutative representations of the Heisenberg group leave symbols of operators unchanged, i.e., $\int_{\mathbb{H}^n} \mathcal{F}^{-1}[\sigma](g)\rho_{h=0}(g)dg = \int\int \mathcal{F}^{-1}[\sigma](p,q)e^{2\pi i(pk+qx)}dpdq = \sigma(k,x)$, we deduce that under the commutative representations the p-mechanical equation of motion (8) reduces to the Hamilton equation

$$\frac{\partial}{\partial t}A(k,x) \quad = \quad \{H(k,x), A(k,x)\}. \tag{17}$$

In summary, the Heisenberg group contains the exact quantum and classical descriptions of a system of particles and provides the correspondence principle between the descriptions. We refer the reader to Chapters 1 and 2 of reference [25] for further information on the subject.

3 The Quantum-Classical Equation of Motion

We proceed to derive an equation of motion for a mixed quantum-classical system. In order to do this we look for an abstract mathematical structure that has the same role as the Heisenberg group in the case of the standard quantization. The desired structure can be constructed based on the following observations.

First, we need two sets of observables $\{D, X\}$ and $\{D', X'\}$ corresponding to quantum and classical parts accordingly. We see no reason to assume that an operator from the first set does not commute with an operator from the second set. We do assume that each set has a Planck constant of its own. Then we let the Planck constant of the second set approach zero and obtain the classical limit for the second subsystem leaving the first one quantum. We know that “Planck constants” arise as characters of the center. Therefore, we need a nilpotent Lie group with a two-dimensional center.

This "quantum-classical group" is generated by two sets of variables $\{hD, X\}$ and $\{h'D', X'\}$ satisfying the commutator relations

$$[hD_j, X_k] = -ih\delta_{jk}I, \qquad [h'D'_{j'}, X'_{k'}] = -ih'\delta_{jk}I', \qquad 1 \leq j,k \leq n; \;\; 1 \leq j',k' \leq n'. \quad (18)$$

Other commutators are zero. The group has a two-dimensional center $\mathbb{Z} = \{sI + s'I'; s, s' \in \mathbb{R}\}$. Irreducible representations of a nilpotent Lie group are induced by the characters of the center [26]. For the quantum-classical group the characters are

$$\mu : (z, z') \mapsto \exp(i(hz + h'z')).$$

It is clear that for $hh' \neq 0$ the induced representation coincides with the irreducible representation of $\mathbb{H}^{n+n'}$ on $L_2(\mathbb{R}^{n+n'})$. This corresponds to *purely quantum* behavior of both sets of variables (see Definition 1.1). The trivial character $h = h' = 0$ gives the family of one-dimensional representations parameterized by $\mathbb{R}^{2(n+n')}$ and the *purely classical* description. These situations were studied in detail in the previous Section. A new situation appears when $h \neq 0$ and $h' = 0$, which produce quantum behavior for the first set and classical behavior for the second set. (The $h = 0$, $h' \neq 0$ case just permutes the quantum and classical parts.) Figure 2 illustrates these facts. We find that in the topology on the dual to the quantum-classical group the quantum descriptions are dense in the quantum-classical and classical descriptions, and the quantum-classical descriptions are dense in the classical ones.

Consider the quantum-classical case in more detail. The quantum-classical representation is given by

$$\rho_h(p, q, s, p', q', s') \;\; = \;\; e^{2\pi i(s\cdot hI + p\cdot hD + q\cdot X + p'\cdot k' + q'\cdot x')}. \quad (19)$$

where $k', x' \in \mathbb{R}^{n'}$ and $h \in \mathbb{R} \setminus \{0\}$. In this representation an element of the convolution algebra on the quantum-classical group is identified with a quantum-classical operator acting of $L_2(\mathbb{R}^n) \otimes \mathbb{R}^{2n'}$. The operator can be computed in terms of the Weyl transform of its symbol

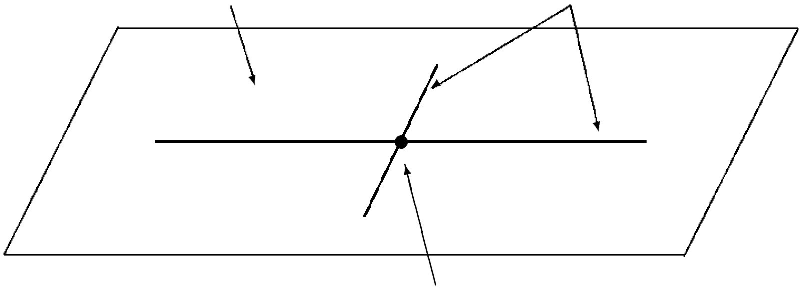

Figure 2: Different types of descriptions generated by a step two nilpotent Lie group with a two-dimensional center.

taken with respect of the quantum (unprimed) coordinates

$$\sigma(hD, X, k', x')f(x) = \int K_\sigma(x, y, k', x')f(y)dy \tag{20}$$

$$K_\sigma(x, y, k', x') = h^{-n}\int \sigma(k, \frac{x+y}{2}, k', x')e^{2\pi i(x-y)k/h}dk. \tag{21}$$

The quantum-classical analog of the commutator is determined by the limiting procedure $h \neq 0$, $h' \to 0$ used to derive the Poisson bracket from the quantum commutator. First we need to obtain the expression for the symbol of the product of two operators. We start with the expression analogous to Eq. (12), but having two, rather than one set of coordinates. Focusing on the primed variables, we carry out the transformations identical to those done in deriving Eq. (16):

$$\begin{aligned}
\sigma\sharp_h\tau(k, x, k', x') &= \left(\frac{2}{h}\right)^{2n}\int\!\!\int\!\!\int\!\!\int du\,dv\,d\eta\,d\zeta\, e^{4\pi i[(x-u)(k-\eta)-(x-v)(k-\zeta)]/h} \\
&\times \left(\frac{2}{h'}\right)^{2n'}\int\!\!\int\!\!\int\!\!\int du'dv'd\eta'd\zeta' e^{4\pi i[(x'-u')(k'-\eta')-(x'-v')(k'-\zeta')]/h'} \\
&\times \sigma(\zeta, u, \zeta', u')\tau(\eta, v, \eta', v') \\
&= \left(\frac{2}{h}\right)^{2n}\int\!\!\int\!\!\int\!\!\int du\,dv\,d\eta\,d\zeta\, e^{4\pi i[(x-u)(k-\eta)-(x-v)(k-\zeta)]/h} \\
&\times \left(\frac{1}{h'}\right)^{2n'}\int\!\!\int du'dv' e^{4\pi i(v'-u')k'}\mathcal{F}_3^{-1}[\sigma](\zeta, u, v', x'+u'h')
\end{aligned}$$

$$\begin{aligned}
&\times\ \mathcal{F}_3[\tau](\eta, v, u', x'+v'h')\\
&=\ \left(\frac{2}{h}\right)^{2n}\iiiint du\,dv\,d\eta\,d\zeta\, e^{4\pi i[(x-u)(k-\eta)-(x-v)(k-\zeta)]/h}\\
&\times\ \sum_{j=0}^{\gamma}\frac{(i\pi h')^j}{j!}[D_{k',\sigma(\zeta,u,k',x')}D_{x',\tau(\eta,v,k',x')}-D_{k',\tau(\zeta,u,k',x')}D_{x',\sigma(\eta,v,k',x')}]^j\\
&\times\ [\sigma(\zeta,u,k',x')\tau(\eta,v,k',x')]+O(h'^{\gamma}).
\end{aligned}\tag{22}$$

At this point it is safe to drop the explicit dependence of the symbols on the primed variables, since the non-commuting nature of the symbols is accounted for by the unprimed variables alone. By taking the limit $h' \to 0$ we obtain the expression for the symbol of the quantum-classical commutator

$$\begin{aligned}
[\sigma\sharp_h\tau-\tau\sharp_h\sigma](k,x)\ &=\ \left(\frac{2}{h}\right)^{2n}\iiiint du\,dv\,d\eta\,d\zeta\, e^{4\pi i[(x-u)(k-\eta)-(x-v)(k-\zeta)]/h}\\
&\times\ \{\sigma(\zeta,u)\tau(\eta,v)-\tau(\zeta,u)\sigma(\eta,v)\\
&+\ \lim_{h'\to 0}\frac{h}{h'}\sum_{j=0}^{\infty}\frac{(-1)^j(\pi h')^{2j+1}}{(2j+1)!}[D_{k',\sigma(\zeta,u)}D_{x',\tau(\eta,v)}\\
&-\ D_{k',\tau(\zeta,u)}D_{x',\sigma(\eta,v)}]^{(2j+1)}[\sigma(\zeta,u)\tau(\eta,v)-\tau(\zeta,u)\sigma(\eta,v)]\}
\end{aligned}\tag{23}$$

or

$$\begin{aligned}
[\sigma,\tau]_{\sharp_h}(k,x)\ &=\ \left(\frac{2}{h}\right)^{2n}\iiiint du\,dv\,d\eta\,d\zeta\, e^{4\pi i[(x-u)(k-\eta)-(x-v)(k-\zeta)]/h}\\
&\times\ \Big[\sigma(\zeta,u)\tau(\eta,v)-\tau(\zeta,u)\sigma(\eta,v)\\
&+\ \frac{ih}{2\pi}\Big(\frac{\partial\sigma(\zeta,u)}{\partial k'}\frac{\partial\tau(\eta,v)}{\partial x'}-\frac{\partial\tau(\zeta,u)}{\partial k'}\frac{\partial\sigma(\eta,v)}{\partial x'}\Big)\Big].
\end{aligned}\tag{24}$$

Eq. (24) for the symbol of the commutator, together with the rule for calculating operators from their symbols given by Eqs. (20) and (21), leads to the following equation of motion for a mixed quantum-classical system

$$\frac{\partial}{\partial t}A(hD,X,k',x')\ =\ \frac{2\pi i}{h}[H,A]_{\sharp_h}(hD,X,k',x').\tag{25}$$

This formula determines the evolution of operator A, which depends on quantum and classical position and momentum variables and acts on $L^2(\mathbb{R}^n) \otimes \mathbb{R}^{2n}$. The kernel of the operator with respect to the $L^2(\mathbb{R}^n)$ subspace is given by Eq. (21).

The quantum-classical equation of motion (25) exhibits many desired features. If A and H depend solely on quantum or classical variables, Eq. (25) reduces to the corresponding purely quantum and purely classical equations, Eqs. (13) and (17) respectively. Since the quantum-classical bracket of the right side of Eq. (25) was obtained by selecting a representation for the Lie bracket of a Lie group, it has all the properties of Lie brackets, in particular, it is antisymmetric and satisfies the Jacobi identity. It is antisymmetric because its symbol is antisymmetric: the integrand of Eq. (24) changes sign under the permutation $\sigma \leftrightarrow \tau$. To prove that the quantum-classical bracket satisfies the Jacobi identity we consider the expression for the symbol of the product of three operators $\sigma(hD, X, k', x')\tau(hD, X, k', x')\phi(hD, X, k', x')$ By successive application of Eq. (22) we get

$$
\begin{aligned}
\sigma\sharp_h\tau\sharp_h\phi(k,x) &= \left(\frac{2}{h}\right)^{2n}\int\!\!\int\!\!\int\!\!\int du_1 dv_1 d\eta_1 d\zeta_1 e^{4\pi i[(x-u_1)(k-\eta_1)-(x-v_1)(k-\zeta_1)]/h}\\
&\times \left(\frac{2}{h'}\right)^{2n}\int\!\!\int\!\!\int\!\!\int du dv d\eta d\zeta[\sigma(\zeta,u)\tau(\eta,v)-\tau(\zeta,u)\sigma(\eta,v)]\\
&\times \Big\{[e^{4\pi i[(\zeta_1-u)(u_1-\eta)-(\zeta_1-v)(u_1-\zeta)]/h}\phi(\eta_1,v_1)\\
&- e^{4\pi i[(\eta_1-u)(v_1-\eta)-(\eta_1-v)(v_1-\zeta)]/h}\phi(\zeta_1,u_1)]\\
&+ i\pi h'\{[D_{k'}\sigma(\zeta,u)\tau(\eta,v)+\sigma(\zeta,u)D_{k'}\tau(\eta,v)\\
&- D_{k'}\tau(\zeta,u)\sigma(\eta,v)-\tau(\zeta,u)D_{k'}\sigma(\eta,v)]\\
&\times e^{4\pi i[(\zeta_1-u)(u_1-\eta)-(\zeta_1-v)(u_1-\zeta)]/h}D_{x'}\phi(\eta_1,v_1)\\
&- e^{4\pi i[(\eta_1-u)(v_1-\eta)-(\eta_1-v)(v_1-\zeta)]/h}D_{k'}\phi(\zeta_1,u_1)\\
&\times [D_{x'}\sigma(\zeta,u)\tau(\eta,v)+\sigma(\zeta,u)D_{x'}\tau(\eta,v)\\
&- D_{x'}\tau(\zeta,u)\sigma(\eta,v)-\tau(\zeta,u)D_{x'}\sigma(\eta,v)]\}+O(h'^2)\Big\}.
\end{aligned}
\tag{26}
$$

After taking the limit $\lim_{h'\to 0}\frac{h}{h'}$ of the first and higher order terms in h' and performing the integrations, this cumbersome expression can be rewritten in a more compact symbolic form as

$$\begin{aligned} \sigma\sharp\tau\sharp\phi &= \sigma\tau\phi - \phi\tau\sigma + i(\sigma_{k'}\tau\phi_{x'} + \sigma\tau_{k'}\phi_{x'} - \tau_{k'}\sigma\phi_{x'} - \tau\sigma_{k'}\phi_{x'} \\ &\quad -\phi_{k'}\sigma_{x'}\tau - \phi_{k'}\sigma\tau_{x'} + \phi_{k'}\tau_{x'}\sigma + \phi_{k'}\tau\sigma_{x'}), \end{aligned} \tag{27}$$

where the subscripts k' and x' indicate differentiation with respect to these variables, and the ordering of the symbols is to be kept track of. Given Eq. (27) it is straightforward to check that the Jacobi identity holds for the symbols of operators: $[[\sigma,\tau]_{\sharp_h},\phi]_{\sharp_h}(k,x,k',x')$, and, therefore, for the quantum-classical bracket.

We used the Weyl correspondence principle to link quantum and classical mechanics and to derive the quantum-classical equation of motion. It is well known, however, that the Weyl correspondence in not unique in mapping phase space functions to Hilbert space operators. In fact, there exist arbitrary many such mappings, differing in the order assigned to products of position and momentum operators. The Weyl rule leads to symmetrized products. For example, it maps kx to $\frac{1}{2}(hD\cdot X + X\cdot hD)$. Another variant of the correspondence principle, widely used in the mathematics community because of its simpler form, is due to Kohn and Nirenberg. It keeps momentum operators on the right, mapping kx to $X\cdot hD$. It is straightforward to obtain a mixed quantum-classical equation of motion using the Kohn-Nirenberg calculus. One starts with $\rho_h = e^{2\pi i q\cdot X}e^{2\pi i p\cdot hD}$ instead of $\rho_h = e^{2\pi i(p\cdot hD + q\cdot X)}$ and follows the same steps. The result is

$$\frac{\partial}{\partial t}A(hD,X,k',x') = \frac{2\pi i}{h}[H,A]^{KN}_{\sharp_h}(hD,X,k',x') \tag{28}$$

with the correspondence rule

$$\begin{aligned} \sigma(hD,X,k',x')^{KN}f(x) &= \int K^{KN}_{\sigma}(x,y,k',x')f(y)dy, \\ K^{KN}_{\sigma}(x,y,k',x') &= h^{-n}\int \sigma(k,x,k',x')e^{2\pi i(x-y)k/h}dk \end{aligned} \tag{29}$$

and the following formula for the quantum-classical bracket of two symbols

$$[\sigma,\tau]^{KN}_{\sharp_h}(k,x,k',x') = \left(\frac{2}{h}\right)^{2n}\int\int dudv e^{4\pi i(x-u)(v-k)/h}\Big\{\sigma(v,x)\tau(k,u) - \tau(v,x)\sigma(k,u)$$

$$+ \quad \frac{ih}{2\pi}\Big[\frac{\partial\sigma(v,x)}{\partial k'}\frac{\partial\tau(k,u)}{\partial x'} - \frac{\partial\tau(v,x)}{\partial k'}\frac{\partial\sigma(k,u)}{\partial x'}\Big]\Big\}. \tag{30}$$

These expressions are somewhat simpler than those obtained by the Weyl correspondence. Eqs. (20,21) and (24,25) are preferable, however, as they preserve the simplectic invariance of the phase space variables and lead via the Wigner transform from the density matrix to the quantum quasi-probability function that is closest to the classical probability density [27].

4 Quantum-Classical Coupling for Harmonic Oscillators

The standard quantization can also be obtained by application of a projection to the classical system under consideration, which leads to a simple description of harmonic oscillators. We briefly summarize this topic and apply it to the case of coupled quantum and classical oscillators. Further information can be found in [28, 29, 30, 31, 32, 33, 34] and references therein.

Let $L_2(\mathbb{C}^n, d\mu_n)$ be a space of functions on $\mathbb{C}^n$ square-integrable with respect to the Gaussian measure

$$d\mu_n(z) = \pi^{-n}e^{-z\cdot\bar{z}}dv(z),$$

where $dv(z) = dxdy$ is the Euclidean volume measure on $\mathbb{C}^n = \mathbb{R}^{2n}$. The Segal-Bargmann [35, 36] (or Fock) space $F_2(\mathbb{C}^n)$ is the subspace of $L_2(\mathbb{C}^n, d\mu_n)$ consisting of all entire functions, i.e., functions $f(z)$ that satisfy

$$\frac{\partial f}{\partial \bar{z}_j} = 0, \qquad 1 \leq j \leq n.$$

Denote by P_Q the orthogonal Bargmann projection [35] of $L_2(\mathbb{C}^n, d\mu_n)$ onto the Fock space $F_2(\mathbb{C}^n)$. Then

$$k(q,p) \to T_{k(q+ip)} = P_Q k(q+ip)I \tag{31}$$

defines the Berezin-Toeplitz (anti-Wick) quantization, which maps a function $k(q,p) = k(q+ip)$ on $\mathbb{R}^{2n} = \mathbb{C}^n$ to the Toeplitz operator T_k. There exists an identification between Berezin and Weyl quantizations [28, 31, 34]. The identification has an especially transparent form for the observables depending only on p or q.

The Berezin-Toeplitz quantization is related to the Heisenberg group more intuitively than the representation of Eq. (4). On a geometrical level, consider the group of Euclidean shifts $a : z \mapsto z+a$ of $\mathbb{C}^n$. To obtain unitary operators on $L_2(\mathbb{C}^n, d\mu)$ the shifts are multiplied by the weight function

$$a : f(z) \mapsto f(z+a)e^{-z\bar{a}-a\bar{a}/2}. \tag{32}$$

This mapping determines [37] a unitary representation of the $(2n+1)$-dimensional Heisenberg group acting on $L_2(\mathbb{C}^n, d\mu)$. The mapping preserves the Fock space $F_2(\mathbb{C}^n)$, and hence all operators of the Eq. (32) form commute with P_Q. The operators are generated by infinitesimal displacements

$$i\sum_{k=1}^{n}\left(a'_j(\frac{\partial}{\partial z'_j} - z'_j - iz''_j) + a''_j(\frac{\partial}{\partial z''_j} - z''_j + iz'_j)\right),$$

where $a = (a_1, \ldots, a_n), z = (z_1, \ldots, z_n) \in \mathbb{C}^n$ and $a_j = (a'_j, a''_j), z = (z'_j, z''_j) \in \mathbb{R}^2$. The generators form a linear space with the basis

$$A_j^{f'} = \frac{1}{i}\left(\frac{\partial}{\partial z'_j} - z'_j - iz''_j\right), \quad A_j^{f''} = \frac{1}{i}\left(\frac{\partial}{\partial z''_j} - z''_j + iz'_j\right). \tag{33}$$

The basis vectors commute with the Bargmann projector P_Q. The operators

$$X_j^{f'} = \frac{1}{i}\left(\frac{\partial}{\partial z'_j} - z'_j + iz''_j\right), \quad X_j^{f''} = \frac{1}{i}\left(\frac{\partial}{\partial z''_j} - z''_j - iz'_j\right) \tag{34}$$

commute with the basis vectors, and we anticipate that P_Q produces a self-adjoint representation of convolutions with respect to $X_j^{f'}$, $X_j^{f''}$, and unit operators. Indeed,

Proposition 3 [21] *The Bargmann projector P_Q defines a representation of convolutions induced by the Weyl-Heisenberg Lie algebra $\mathfrak{h}_n$ operating on $\mathbb{C}^n$ by* Eqs. (34). *The kernel $b(t, \zeta), t \in \mathbb{R},\ zeta \in \mathbb{C}^n$ of the representation is given by the formula*

$$\widehat{b}(t, \zeta) = 2^{n+1/2}e^{-1}e^{-(t^2+\zeta\bar{\zeta}/2)}.$$

We move on to apply the Bargmann projection technique to the quantum-classical coupling of harmonic oscillators.

Example 4 [30] In the Segal-Bargmann representation the operators of creation and annihilation of the jth state of a particle are $a_j^+ = z_j I$ and $a_j^- = \partial/\partial z_j$, correspondingly. Consider an n degree of freedom harmonic oscillator with the classical Hamilton function

$$H(q,p) = \frac{1}{2}\sum_{j=1}^{n}(q_j^2 + p_j^2).$$

The corresponding quantum Hamiltonian is obtained by the Bargmann projection

$$T_{H(q,p)} = \frac{1}{2}P_Q \sum_{j=1}^{n}(q_j^2 + p_j^2)I = \frac{1}{2}(nI + \sum_{j=1}^{n} z_j \frac{\partial}{\partial z_j}). \tag{35}$$

The right side of Eq. (35) is the celebrated Euler operator. It generates the well known dynamical group [38, Chap. 1, Eq. (6.35)]

$$e^{itT_{H(p,q)}} f(z) = e^{int/2} f(e^{it} z), \qquad f(z) \in F_2, \tag{36}$$

which induces rotation of the $\mathbb{C}^n$ space. The evolution of the classical oscillator is also given by a rotation, that of the phase space $\mathbb{R}^{2n}$

$$z(t) = G_t z_0 = e^{it} z_0, \qquad z(t) = p(t) + iq(t),\ z_0 = p_0 + iq_0. \tag{37}$$

The projection P_Q leads to the Segal-Bargmann representation, providing a very straightforward correspondence between quantum and classical mechanics of oscillators, in contrast to the rather complicated case of the Heisenberg representation [38, Prop. 7.1 of Chap. 1].

The powers of z are the eigenfunctions $\phi_n(z) = z^n$ of the Hamiltonian (35), and the integers n are the eigenvalues. Either pure or mixed, any initial state of the oscillator remains unchanged during the Eq. (36) evolutions and no transitions are observed.

Now consider classical and quantum oscillators coupled by a quadratic term

$$H(p,q;p',q') = \frac{1}{2}(p'^2 + p^2 + x'^2 + x^2 + \alpha(x' - x)^2). \tag{38}$$

Applying the canonical transformation (see [39, § 23.D])

$$q' = \frac{q_1 + q_2}{\sqrt{2}}, \qquad q = \frac{q_1 - q_2}{\sqrt{2}}, \qquad p' = \frac{p_1 + p_2}{\sqrt{2}}, \qquad p = \frac{p_1 - p_2}{\sqrt{2}}, \tag{39}$$

or, equivalently, introducing complex variables $z = q + ip$, $z' = q' + ip'$, $z_1 = q_1 + ip_1$, $z_2 = q_2 + ip_2$

$$\begin{aligned} z' &= \frac{z_1 + z_2}{\sqrt{2}}, \qquad z = \frac{z_1 - z_2}{\sqrt{2}}, \\ z_1 &= \frac{z' + z}{\sqrt{2}}, \qquad z_2 = \frac{z' - z}{\sqrt{2}}, \end{aligned} \tag{40}$$

we get rid of the coupling term

$$H(p_1, q_1; p_2, q_2) = \frac{1}{2}(p_1^2 + p_2^2 + \omega_1^2 q_1^2 + \omega_2^2 q_2^2), \tag{41}$$

where $\omega_1 = 1$, $\omega_2 = \sqrt{1 + 2\alpha}$. The two uncoupled oscillators evolve independently

$$z_1(t) = e^{2i\omega_1 t} z_1(t_0), \qquad z_2(t) = e^{2i\omega_2 t} z_2(t_0)$$

The dynamics in the original coordinates, however, is not trivial. The primed and unprimed (quantum and classical) variables mix

$$z'(t) = \frac{(e^{2i\omega_1 t} + e^{2i\omega_2 t}) z'(t_0) + (e^{2i\omega_1 t} - e^{2i\omega_2 t}) z(t_0)}{2}, \tag{42}$$

$$z(t) = \frac{(e^{2i\omega_1 t} - e^{2i\omega_2 t}) z'(t_0) + (e^{2i\omega_1 t} + e^{2i\omega_2 t}) z(t_0)}{2}. \tag{43}$$

Suppose that the classical subsystem is initially localized at a point z_0' the phase space and the quantum subsystem is in its n-th pure state $\phi(z', z; t_0) = \delta(z_0' - z') \otimes z^n$. The dynamics of the combined system is given by

$$\phi(z', z; t) = \delta\left(z_0 - \frac{(e^{2i\omega_1 t} + e^{2i\omega_2 t}) z' + (e^{2i\omega_1 t} - e^{2i\omega_2 t}) z}{2}\right) \tag{44}$$

$$\otimes \left(\frac{(e^{2i\omega_1 t} - e^{2i\omega_2 t}) z' + (e^{2i\omega_1 t} + e^{2i\omega_2 t}) z}{2}\right)^n. \tag{45}$$

During the evolution the classical subsystem, [Eq. (44)] is always sharply supported, i.e. represented by the delta function, while the quantum subsystem, [Eq. (45)] evolves into a mixed state. The binomial (45) contains all powers of z less or equal to n ($z^k, k \leq n$). Therefore, there exists a non-zero probability for the quantum subsystem to make a transition from the initial pure state z^n into a lower energy state z^k, $k < n$. It is remarkable that in this particular case the interaction with the classical subsystem can only decrease the initial energy of the quantum one. The overall dynamics is (quasi)-periodic with the recurrence time determined by the frequencies ω_1 and ω_2.

5 Discussion and Conclusions

The quantum-classical equation of motion (25) can be applied in several ways depending on how one describes the quantum and classical subsystems. The classical subsystem can be treated on the level of trajectories, in which case it is represented by a point in the phase space $\{k'_i, x'_i\}$ evolving according to the Hamilton equations with the quantum-classical bracket of Eq. (24) regarded as a modification of the Poisson bracket. If at the same time the Heisenberg equation of motion with the quantum-classical bracket in place of the commutator is used to describe the evolution of quantum operators, the mean field approximation is recovered. Namely, the quantum mechanical average of Eq. (25) with respect to the wave function Ψ is given by

$$\frac{\partial}{\partial t}\langle\Psi|A(k',x')|\Psi\rangle \quad = \quad \frac{2\pi i}{h}\langle\Psi|[H,A]_{\sharp_h}(k',x')|\Psi\rangle. \tag{46}$$

If A is a purely quantum mechanical observable independent of classical variables, the derivatives $\partial A/\partial k'$ and $\partial A/\partial x'$ in the quantum-classical bracket Eq. (24) vanish, and we obtain

$$\frac{\partial}{\partial t}\langle\Psi|A|\Psi\rangle \quad = \quad \frac{2\pi i}{h}\langle\Psi|[H(k',x'),A]|\Psi\rangle \tag{47}$$

with the Hamiltonian H parametrically depending on the classical phase space variables k' and x'. Substituting the variables in place of $A(k',x')$ in Eq. (46), we recover the classical equations of motion, the classical Hamiltonian being the quantum mechanical average of the total Hamiltonian

$$\begin{aligned}\frac{\partial k'}{\partial t} &= -\frac{\partial \langle \Psi | H(k',x') | \Psi \rangle}{\partial x'}, \\ \frac{\partial x'}{\partial t} &= \frac{\partial \langle \Psi | H(k',x') | \Psi \rangle}{\partial k'}.\end{aligned} \tag{48}$$

Eqs. (47) and (48) constitute the traditional mean field approximation: classical variables are coupled to the expectation values of quantum observables.

The quantum-classical equation of motion can be looked upon in a different way, namely, as a Liouville-von Neumann equation for a mixed distribution $\rho(hD, X, k', x')$. Selecting a quantum basis we get a set of coupled equations for classical phase space distribution functions $\rho_{ij}(k', x')$ corresponding to each pair of the quantum basis states i, j

$$\frac{\partial \rho_{ij}}{\partial t} = \frac{2\pi i}{h} \sum_k \left[H^*_{ik}\rho_{kj} - \rho^*_{ik} H_{kj} + \frac{ih}{2\pi}\left(\frac{\partial H^*_{ik}}{\partial k'} \frac{\partial \rho_{kj}}{\partial x'} - \frac{\partial \rho^*_{ik}}{\partial k'} \frac{\partial H_{kj}}{\partial x'} \right) \right] \tag{49}$$

In the purely quantum and classical limits the two derivatives [Eqs. (47), (48) and Eq. (49)] of the quantum classical equation of motion [Eq. (25)] are equivalent. In the mixed case they are not, because of non-local correlations in the classical subsystem induced by its interaction with the quantum one. Such correlations, inherent in the Liouville-von Neumann equation, do not appear on the level of individual trajectories. In particular, if the equations (49) are integrated with the initial conditions $\rho_{11}(k', x') = \delta(k' - k'_0)\delta(x' - x'_0)$ and $\rho_{ij} = 0$, $\forall \{ij\} \neq \{11\}$, at later times, in general, $\rho_{ij} \neq 0$ because of the couplings $H_{ij} \neq 0$. In other words, classical phase space distribution functions associated with different quantum states differ and mix. Spreading of initially localized classical distributions is enhanced by their mutual mixing. An initially localized phase space distribution ρ_{11} corresponding to the ground quantum state populates excited state distributions. They undergo diverging evolutions, and later, when ρ_{11} gains an admixture of the excited state distributions, it necessarily becomes delocalized. This, of course, can not happen in the mean field approach, where the classical subsystem is described by a single trajectory. Non-local correlations are averaged out in the mean field approximation.

If there is no coupling between quantum states, phase space distributions neither mix nor spread beyond the classical divergence. Consider a purely adiabatic case, where the quantum basis states are the instantaneous eigenstates of the quantum Hamiltonian. In the absence of non-adiabatic coupling Eq. (49) splits into a set of uncoupled equations for classical distribution functions corresponding to individual adiabatic quantum states. An adiabatic evolution of every distribution function can be equivalently described by the classical trajectory mean field approach [Eqs. (47)–(48)] with the wave function Ψ being the corresponding adiabatic eigenstate of the quantum Hamiltonian.

The Liouville-von Neumann equation for the evolution of the mixed distribution reduces to the coupled equations of the mean field approximation if the quantum-classical function is constrained to

$$\rho \;=\; |\Psi\rangle\langle\Psi| \cdot \delta(k'-k'')\delta(x'-x''), \tag{50}$$

where k',k'' and x',x'' are the n-dimensional classical momentum and position vectors. Under this constraint the quantum part of the mixed function always remains a pure state, and the classical part is always represented by a delta function. Substituting expression (50) for ρ in place of A in Eq. (25) and integrating out the phase space variables ($\int dk'' \int dx''$) we obtain the von Neumann equation with the quantum Hamiltonian depending on classical coordinates $H(k', x')$. Since the density matrix entering the equation is constructed from a pure quantum state Ψ, the von Neumann equation for the density matrix is isomorphic to the Schrödinger equation and to Eq. (47). To recover the mean field equations for the classical variables (48) we substitute (50) into (25), multiply both sides by either k' or x', and integrate over quantum and classical coordinates.

The mean field approximation can not reproduce the non-local correlations within the classical subsystem due to interaction with individual parts of the quantum subsystem. At the same time, such correlations naturally appear in the solutions to the Liouville-von Neumann equation. Unfortunately, the Liouville-von Neumann equation does not provide significant computational advantage over the pure quantum von-Neumann equation, since both deal with delocalized distributions. On the other hand, propagation of an individual classical trajectory via the Hamilton equations of motion is far less demanding than integration of the Liouville equation. The idea of running and then averaging over a few representative trajectories instead of propagating the total phase space distribution function is fully exploited in classical molecular dynamics simulations (see, for instance, reference [40]). In order to account for the quantally induced non-local correlations among the phase space variables, while retaining a trajectory description for the classical subsystem, we interpolate between the mean field and Liouville-von Neumann approaches by developing a multiconfiguration version of the mean field method. We start with the quantum-classical distribution function

$$\rho \;=\; \sum_i \sum_j \varrho_{ij} |\Psi_i\rangle\langle\Psi_j| \cdot \delta(k'_{ij} - k')\delta(x'_{ij} - x'), \tag{51}$$

where the sums run over the number of independent configurations. Taking the wave functions to be orthonormal $\langle\Psi_i|\Psi_j\rangle = \delta_{ij}$ we substitute (51) into Eq. (25) and integrate over the classical variables ($\int dk' \int dx'$) to obtain the von Neumann equation for the quantum density matrix $\varrho = \sum_i \sum_j \varrho_{ij}|\Psi_i\rangle\langle\Psi_j|$

$$\frac{\partial \varrho_{ij}}{\partial t} \;=\; \frac{2\pi i}{h} \sum_k [H^*_{ik}(k'_{ik}, x'_{ik})\varrho_{ik} - \varrho^*_{kj} H_{kj}(k'_{kj}, x'_{kj})]. \tag{52}$$

To get the equations of motion for the classical variables k_{ij}, x_{ij} we substitute (51) into Eq. (25), multiply both sides by the corresponding variable, and integrate over all degrees of freedom. We obtain equations of motion for the "diagonal" positions and momenta as

$$\begin{aligned} \frac{\partial k'_{ii}}{\partial t} &= -\sum_k \frac{\partial H_{ki}(k'_{ki}, x'_{ki})}{\partial x'_{ki}}, \\ \frac{\partial x'_{ii}}{\partial t} &= \sum_k \frac{\partial H^*_{ik}(k'_{ik}, x'_{ik})}{\partial k'_{ik}} = \sum_k \frac{\partial H_{ki}(k'_{ki}, x'_{ki})}{\partial k'_{ki}}. \end{aligned} \tag{53}$$

The corresponding expressions for the "non-diagonal" variables are more complicated

$$\frac{\partial x'_{ij}}{\partial t} \;=\; \sum_k H^*_{ik}(k_{ik}, x_{ik}) x'_{kj} - x'_{ik} H_{kj}(k_{ik}, x_{ik}) + \frac{\partial H_{ik}(k_{ik}, x_{ik})}{\partial k'_{ik}}, \tag{54}$$

and similarly for momenta. In order to keep the Hamiltonian matrix $\| H_{ij}(k'_{ij}, x'_{ij}) \|$ hermitian we require that the position and momentum "matrices" are symmetric: $k'_{ij} = k'_{ji}$, $x'_{ij} = x'_{ji}$. With this constraint the "non-diagonal" evolutions simplify, the first two terms in formula (54) disappear, and the dynamics of the "non-diagonal" phase space variables coincide with the average dynamics of the "diagonal" variables

$$\begin{aligned}
\frac{\partial x'_{ij}}{\partial t} &\equiv \frac{1}{2}\Big(\frac{\partial x'_{ij}}{\partial t} + \frac{\partial x'_{ji}}{\partial t}\Big) \\
&= \frac{1}{2}\sum_k \Big(H^*_{ik}x'_{kj} - x'_{ik}H_{kj} + \frac{\partial H_{ik}}{\partial k'_{ik}} + H^*_{jk}x'_{ki} - x'_{jk}H_{ki} + \frac{\partial H_{jk}}{\partial k'_{jk}}\Big) \\
&= \frac{1}{2}\sum_k \Big(\frac{\partial H_{ik}}{\partial k'_{ik}} + \frac{\partial H_{jk}}{\partial k'_{jk}}\Big) = \frac{1}{2}\Big(\frac{\partial x'_{ii}}{\partial t} + \frac{\partial x'_{jj}}{\partial t}\Big), \\
\frac{\partial k'_{ij}}{\partial t} &= \frac{1}{2}\Big(\frac{\partial k'_{ii}}{\partial t} + \frac{\partial k'_{jj}}{\partial t}\Big).
\end{aligned} \tag{55}$$

Apart from assigning the "non-diagonal" coordinates and momenta unique values a simple physical meaning: $x'_{ij} = (x'_{ii} + x'_{jj})/2$, $k'_{ij} = (k'_{ii} + k'_{jj})/2$, Eqs. (55) reduce the number of independent classical trajectories in the n-dimensional multiconfiguration mean field approximation from n^2 to n.

The idea of introducing multiple configurations is not new. Apparently, it originated in quantum chemistry as an improvement on the self-consistent field solution of the time independent Schrödinger equation. The time dependent fully quantum multiconfiguration self-consistent field approach is discussed in reference [41]. Equations of motion similar to our version of the quantum-classical multiconfiguration approximation were proposed by Diestler [5]. The method was devised to account for non-local correlations among the classical degrees of freedom of a condensed phase solvent interacting with a quantum solute. Our approach has a different derivation and is less computationally demanding by a factor of n. The number of configurations in the multiconfiguration mean-field method does not have to be the same as the number of quantum (adiabatic) basis states. The former is usually less than the latter, and, in the case when the classical phase space can be separated into a union of several weakly connected regions, it should be determined by the number of such regions. For example, a double well system would require two configurations — two classical trajectories, each originating in its own well.

The quantum-classical equation of motion is derived here via the simplest extension of the Heisenberg group of quantum and classical mechanics to the group allowing for two sets of variables, such that the variables of the first set do not commute, while the variables of the second set do. Obviously, there exist other groups satisfying this requirement. It is possible, for instance, to consider a step three nilpotent Lie group and the corresponding algebra decomposable as a vector space into the three subspaces V_0, V_1, and V_2 having the following properties: The elements of V_0 commute with all elements and form the center. Commutators of vectors from V_1 belong to V_0. Commutators of vectors from V_2 belong to V_1. By taking a representation of this group that maps the center V_0 to zero, we would obtain another model for a mixed quantum-classical system, where vectors from V_1 would correspond to classical degrees of freedom, since their commutators vanish, while vectors from V_2 would describe quantum variables. It is likely, though, that this scheme will exhibit properties atypical for quantum and classical mechanics, since step three nilpotent Lie groups differ from step two groups and the Heisenberg group in particular. There exist, however, some advantages in dealing with general nilpotent Lie groups. For example, the relativistic quantization considered in reference [42] is based on a representation of the simplest step three nilpotent Lie group (*meta Heisenberg group* [43]) spanned by the Schrödinger representation of the Heisenberg group and the operators of multiplication by functions. Application of the quantization rules to the appropriate Lie algebras leads to quantum-classical constructions for string theory, conformal field theory, and Yang-Mills theories [44].

In summary, we presented a systematic approach to coupling quantum and classical degrees of freedom based on a generalization of the unified description of quantum and classical mechanics in terms of convolutions on the Heisenberg group. Considering the simplest extension of the Heisenberg group that allows for two distinct sets of variables, we derived a quantum-classical equation of motion. The quantum-classical bracket entering the equation is a Lie bracket and, therefore, possesses the two most important properties common to the quantum commutator and the Poisson bracket: It is antisymmetric and satisfies the Jacobi identity. We explicitly constructed the quantum-classical equation of motion for coupled harmonic oscillators and discussed approximations to the equations applicable to more general cases.

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