

# Time Dependent Variational Principle and Coherent State Orbits for a Trapped Ion

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## **Abstract.**

Spectral properties of the Hamiltonian function which characterizes a trapped ion are investigated. In order to study semiclassical dynamics of trapped ions, coherent state orbits are introduced as sub-manifolds of the quantum state space, with the Kähler structure induced by the transition probability. The time dependent variational principle is applied on coherent states' orbits. The Hamilton equations of motion on Kähler manifolds of the type of classical phase spaces naturally arise. The associated classical Hamiltonian is obtained from the expected values on symplectic coherent states of the quantum Hamiltonian. Spectral information is thus coded within the phase portrait. We deal with the bosonic realization of the Lie algebra of the  $SU(1,1)$  group, which we particularize for the case of an ion confined in a combined, Paul and Penning trap. This formalism can be applied to Hamiltonians which are nonlinear in the infinitesimal generators of a dynamical symmetry group, such as the case of ions confined in electrodynamic traps. Discrete quasienergy spectra are obtained and the corresponding quasienergy states are explicitly realized as coherent states parameterized by the stable solutions of the corresponding classical equations of motion. A correspondence between quantum and classical stability domains is thus established, using the Husimi representation.

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## 1. Introduction. Classical-quantum correspondence

The development of quantum mechanics and its concepts left it with a heavy legacy of classical concepts. The most notable among them is Bohr's correspondence principle, which states that in the limit of large quantum numbers there are similarities between classical and quantum dynamics. In other words, the results from classical mechanics are *macroscopically correct* and may be regarded as limit cases of the quantum mechanics results, when quantum physics discontinuities are negligible. This principle is still used as an intuitive guide for finding quantum properties which are similar to known classical laws. Some of these analogies are intriguing, considering the fundamental differences in the mathematical formalism underlying the two theories: quantum mechanics uses a separable Hilbert space with a unitary inner product, while classical mechanics is based on a continuous phase space endowed with a symplectic structure [1, 2]. Nevertheless, in certain situations it might represent a weak correspondence between classical and quantum concepts. The concept of observables in quantum mechanics and in classical probability theory has drawn a lot of interest. It was shown that, by means of injective statistical maps, quantum mechanics can to a certain extent be reformulated in classical terms [3].

Pure and mixed states of a  $n$ -dimensional quantum entity can be represented as points of a subset of a  $n^2$  dimensional real space [4]. Mathematically, a pure quantum state is typically represented by a vector in a Hilbert space. Mixed quantum states are characterized by means of density matrices. Both mixed and pure state are intensively investigated, due to a very large interest which they present for modern physics. The expressions *coherent* and *incoherent* superposition of quantum states are also used in order to help distinguish between pure and mixed states. There exist superpositions of quantum states which exhibit many features similar to those of their classical counterparts: they are the so-called coherent states, investigated by Schrödinger in 1926 [5] and then rediscovered by Klauder [6, 7], Glauber [8, 9] and Sudarshan [10] at the beginning of the 1960s. Glauber coined the term 'coherent states' in 1963, in the context of quantum optics [11]. Such states are superpositions of Fock states of the quantized electromagnetic field that, below the limit of a complex factor, are not modified by the action of the photon annihilation operator [12]. Since then, coherent states had a huge impact on quantum physics [13, 14, 15, 16, 17, 18, 19] with widespread applications such as nuclear, atomic and condensed matter physics [20, 21, 22, 23, 24, 25], quantum field theory [26], problems of quantization and dequantization [24, 25, 27], non-commutative quantum mechanics [28] which tries to unify quantum mechanics and gravity, path integrals, signal analysis and recently, quantum information processing (QIP) [23, 24, 25, 29, 30, 31] using the entanglement feature [12, 23, 26, 32, 33]. Moreover, there are a lot of quantum states of interest for modern physics and not only [34], such as Fock states, Schrödinger-cat states [18, 32] or squeezed states [35, 36, 37, 38]. A matter of interest is the engineering of quantum states showing negative parts in their Wigner functions, which is a signature for non-classical properties of the state

that can not be explained using a classical phase-space distribution. All these represent problems of ever increasing interest, because they discuss the relation between classical and quantum physics, of the blurred separation line between the two of them.

A charged particle driven by a time-dependent perturbation in a quantum system is a non-trivial fundamental issue, with numerous applications such as nonlinear dynamics (quantum chaos) [39], quantum simulation of the Dirac equation and implicitly quantum field theories [40, 41], cavity QED [42, 43], quantum non-locality [44], quantum transport [45], quantum optics [19, 46, 47, 48], superpositions of arbitrary quantum states [49] or quantum information processing [32, 33, 50, 51, 52, 53]. The paper investigates quantum dynamics for systems with dynamical symmetry, such as is the case of ions confined in electrodynamic traps or combined (Paul and Penning) traps [54]. The coherent states' orbits are introduced as sub-manifolds of the quantum state space, with a Kähler structure induced by the transition probability. An algorithm was found, which associates a classical Hamiltonian to the quantum Hamiltonian describing the ion. The classical Hamiltonian implicitly contains the spectral information of the quantum system. The coherent states formalism introduced in [55, 56] and developed in [27] is used, and the time dependent variational principle (TDVP) [57, 58, 59], in order to characterize the semiclassical dynamics.

The results have been applied to the case of an ion confined in a quadrupole electromagnetic trap with anharmonicities, in order to study semiclassical dynamics. The coherent states formalism for dynamical groups and the time dependent variational principle (TDVP) are applied with an aim to investigate semiclassical behaviour of trapped ions. The explicit expression of the quantum Hamiltonian associated to a charged particle is found, as a function of the Lie algebra generators for the radial and axial symplectic groups. The Schrödinger equation solution also results. The Hamiltonian function is then particularized to the case of combined, quadrupole and octopole traps.

The paper is organized as follows: Section 2 reviews some of the definitions from the geometry of coherent states. In Section 3 the time dependent variational principle is applied to a manifold of test vectors in paragraph 3.1. The Lagrange function is introduced and the Hamilton equations of motion result for the system we have investigated in Section 3.2. In Section 3.3 we introduce the coherent states built over the weight states of the discrete positive series of the symplectic group  $\mathcal{Sp}(2, \mathbb{R})$  and the Lie algebra generators. A model is proposed which enables the explicit calculus of the Husimi function for every algebraic model with a dynamical group. The equations of motion in phase space are inferred. The model we suggest is applied in Section 4 to a combined, Paul and Penning trap, with octupole anharmonicity. The Lie algebra generators for the radial and axial symplectic group  $\mathcal{Sp}(2, \mathbb{R})_{a,r}$  are introduced in Section 4.1, together with the Hamiltonian of the system. The symplectic coherent states representation is introduced in Section 4.3. The classical Hamiltonian for the system we investigated is finally obtained. Section 5 is dedicated to a discussion of the results.

## 2. Coherent states for dynamical symmetry groups

### 2.1. Notions of differential geometry

Euclidian space is a basic symplectic manifold, not only because it is simple to characterize, but mainly to the fact that it provides a local model for every symplectic manifold. The Euclidean space can be treated as a semi-local symplectic manifold. Hence we can submit global nonlinear problems on it. The phase space is a space endowed with a tensor, which gives it the geometric structure. It is called a symplectic form. Symplectic manifolds are even-dimensional. They are studied using symplectic geometry or symplectic topology [60, 61], which represents a branch of differential geometry (topology) [62]. Symplectic manifolds arise naturally in abstract formulations of classical mechanics and analytical mechanics as the cotangent bundles of manifolds, e.g. in the Hamiltonian formulation of classical mechanics [60, 63]. The subject of symplectic topology is the global structure of a symplectic manifold and the behaviour of symplectomorphisms which are far from identity. These aspects are of interest both in Euclidean space with its associated standard linear symplectic structure and on general symplectic manifolds [61, 62]. A Kähler manifold is a symplectic manifold with an integrable almost complex structure. A consequence of the integrability theorem is the fact that every Riemann surface carries a Kähler structure [64]. Most symplectic manifolds are not Kähler, which means they do not possess an integrable complex structure compatible with the symplectic form. Gromov [65, 66] made the important observation that symplectic manifolds admit an abundance of compatible almost complex structures, so that they satisfy all the axioms for a Kähler manifold except the requirement that the transition functions be holomorphic. Any real valued differential function  $H$  on a symplectic manifold can serve as an energy function or Hamiltonian.

### 2.2. Coherent states geometry

Further on, we will recall some definitions and constructions from the geometry of coherent states [13, 14, 29], while introducing the elementary quantum systems (in the Wigner sense), which represent the most extended class of models describing both analytically and numerically the energetic spectra and the solutions of the Schrödinger equation.

Let  $G$  be a Lie group acting on a manifold  $M$  (respectively, a complex Lie group acting on a complex manifold  $M$ ). Then for every point  $m \in M$  we define its *orbit* by  $\mathcal{O}_m = G_m = \{g.m | g \in G\}$  and stabilizer by [67]

$$G_m = \{g \in G | g.m = m\} \quad (1)$$

We will denote by  $\mathcal{H}$  the separable complex Hilbert space of the state vectors (quantum states). The state space in quantum mechanics will be denoted by  $\mathcal{P}(\mathcal{H})$ . If  $\psi \in \mathcal{H}$  is a state vector, then  $\hat{\psi} = \{\lambda\psi | \lambda \in \mathbb{C}\}$  represents the state associated to  $\psi$ .

Then

$$\mathcal{P}(\mathcal{H}) = \left\{ \hat{\psi} \mid \psi \in \mathcal{H} \setminus \{0\} \right\}, \quad (2)$$

is the state space, which is also a projective complex space.  $\hat{\psi}$  is an unidimensional, complex linear space. If using normalized states ( $\|\psi\| = 1$ ), we can introduce the states as radii and we have  $\hat{\psi} = \left\{ e^{i\varphi} \cdot \psi \mid \varphi \in \mathbb{R} \right\}$ . In the following, we will consider  $\mathcal{U}$  as an irreducible unitary representation of the Lie group  $\mathcal{G}$  in  $\mathcal{H}$ . This means that  $\mathcal{U}(g)$  is a unitary operator on  $\mathcal{H}$  for  $\forall g \in \mathcal{G}$ , such as

$$\mathcal{U}(g \cdot g') = \mathcal{U}(g) \cdot \mathcal{U}(g'), \quad \forall g, g' \in \mathcal{G}$$

$$\mathcal{U}(g^{-1}) = [\mathcal{U}(g)]^{-1} = \mathcal{U}^+(g) .$$

where  $\mathcal{U}^+$  is the adjoint of  $\mathcal{U}$ . This representation induces an action of the group  $\mathcal{G}$  on  $\mathcal{P}(\mathcal{H})$ , defined as  $g\hat{\psi} = \widehat{\mathcal{U}(g)\psi}$  for  $\forall g \in \mathcal{G}$  and  $\psi \in \mathcal{H} \setminus \{0\}$ . Then  $\mathcal{G}_0$  is the *stationary group* of the state  $\hat{\psi}$ , defined as

$$\mathcal{G}_0 = \left\{ g \mid g \cdot \hat{\psi} = \hat{\psi}, \quad g \in \mathcal{G} \right\}$$

The orbit  $\mathcal{G} \cdot \hat{\psi} = \left\{ g \cdot \hat{\psi} \mid g \in \mathcal{G} \right\}$  is called a coherent state orbit, while any state  $g \cdot \hat{\psi}$  is called a *coherent state* for the group  $\mathcal{G}$ . We will denote  $\mathcal{O}_{\hat{\psi}} = \mathcal{G} \cdot \hat{\psi}$ . The *coherent vectors* which determine the coherent states, can be parametrized with the coordinates of the quotient space  $\mathcal{M} = \mathcal{G}/\mathcal{G}_0$ . For a large class of symmetry groups  $\mathcal{G}$ ,  $\mathcal{M}$  presents a structure of classical phase space (symplectic manifold). Thus it is convenient to parametrize the try functions with points from  $\mathcal{M}$ . There exists a bijection between the points from  $\mathcal{M}$ , considered as classical states, and the coherent states.

The triplet  $(\mathcal{H}, \mathcal{U}, \mathcal{G})$  is defined as an *elementary quantum system* in the Wigner sense or a *quantum system with symmetry*, where  $\mathcal{H}$  is a separable Hilbert space,  $\mathcal{G}$  is a group and  $\mathcal{U}$  stands for an irreducible unitary representation. Coherent states can be associated with such systems. We will consider that the orbit  $\mathcal{O}_{\hat{\psi}}$  is a sub-manifold of the space  $\mathcal{P}(\mathcal{H})$  with a structure of Kähler space induced by the transition probability. Coherent state Kähler orbits are obtained for Heisenberg groups, compact groups and semisimple groups, with representations belonging to the holomorphic discrete series. The coherent states considered here have important applications in quantum physics and quantum optics, especially when referring to the physics of trapped atomic particles.

Thus a family of coherent states provides the opportunity of investigating the quantum world using the methods of study applied to the classical world. This feature allowed Glauber and others to treat a quantized boson or fermion field as a classical field, with an aim to compute correlation functions and other quantities relevant for statistical physics, such as partition functions. Hence, the system can be characterized by means of the associated classical trajectories.

### 2.3. $SU(1,1)$ group in quantum optics

We now turn our attention to elements of the group theory, especially those related to the  $SU(1,1)$  group, which presents a great interest for this paper. A. O. Barut and L. Girardello [68], then A. M. Perelomov [13, 14] have brought in the  $SU(1,1)$  group to quantum optics. They have constructed the coherent states of the  $SU(1,1)$  group in different space representations: Hilbert space and unit disk space or Lobachevian space [14, 69]. We will focus on geometrical aspects of coherent states and generalized coherent ones, based on Lie algebras, especially on the  $\mathfrak{su}(1,1)$  Lie algebra [70, 71, 72, 73]. The topological space that parametrizes the elements of a Lie group is a manifold. We can ascertain that a Lie group is a finite dimensional manifold.

Generally, group methods are used in order to find degenerate states of a given state in quantum mechanics [74, 75]. The Lie algebra of the generalized special unitary group  $SU(1,1)$  is widely used in quantum optics. The  $SU(1,1)$  coherent states arise in the case of generation of boson pairs with zero spins in homogeneous alternating electric field or in the gravitation field of the expanding Universe [76]. In particular Wódkiewicz and Eberly [77] have discussed the role of the generalized coherent states of Perelomov [13, 14] associated with the Lie algebra of the  $SU(1,1)$  group in connection with variance reduction. Applications of this group are tightly connected with squeezed states of light. Coherence-preserving Hamiltonians associated with the  $SU(1,1)$  generalized coherent states have been studied by Gerry [79, 80]. It should be emphasized that the  $SU(1,1)$  generalized coherent states in [13] and [77] are special cases of the two-photon coherent states discussed by Yuen [38]. This fact has been used by Gerry [79, 80] who applied the  $SU(1,1)$  formulation of the two-photon coherent states to the issue of the interaction of squeezed light with a nonlinear non-absorbing medium modelled as an anharmonic oscillator. The coherent states have been especially useful in quantum optics and quantum information processing (QIP) [12, 23, 24]. Each mode of the electromagnetic field may be formally described as a harmonic oscillator, and different quantum states of the oscillator correspond to different states of the field. The field from a single-mode laser operating far enough above threshold can be described for many purposes as a coherent state; it differs from a coherent state in that its phase drifts randomly. Coherent states also play an important role in mathematical physics [12, 14, 69, 73]. In the present paper we will study the bosonic realization of the Lie algebra for the  $SU(1,1)$  group.

The  $SU(1,1)$  group [12] consists of unimodular matrices of  $2 \times 2$  dimension with unit determinant. It is also isomorphic to the following noncompact groups [81]:

$$SO(2,1) \approx SU(1,1) \approx SL(2, \mathbb{R}) \approx Sp(2, \mathbb{R}). \quad (3)$$

For example, we can construct the three-dimensional noncompact group  $SU(1,1)$  by taking the intersection of the unitary group  $U(1,1)$  with  $SL(2; \mathbb{C})$ . All usual groups of linear algebra such as  $GL(n, \mathbb{R})$ ,  $SL(n, \mathbb{R})$ ,  $O(n, \mathbb{R})$ ,  $U(n)$ ,  $SO(n, \mathbb{R})$ ,  $SU(n)$ ,  $Sp(n, \mathbb{R})$  are real or complex Lie groups [67].

### 3. The Variational Principle

#### 3.1. The Variational Principle. Test states

The equations of motion in classical mechanics arise as solutions of variational problems. An example would be Fermat's principle of least time, stating that light propagates between two points by a path which takes the shortest possible amount of time. In a manner similar to light, all systems possessing only kinetic energy move along geodesics, which are paths minimizing energy. A general mechanical system possesses both kinetic and potential energy. In such case the quantity which is minimized is the mean value of the difference between the kinetic and potential energy. This less intuitive quantity is called the action [61]. The variational principle results from the definition of an action integral  $S = \int_{t_1}^{t_2} L(\psi) dt$ , where the real Lagrange function of this variational problem is defined as [57, 62]

$$L(\psi) = \frac{1}{\langle \psi | \psi \rangle} \left[ \langle \psi | H | \psi \rangle - \Im m \left\langle \frac{\partial \psi}{\partial t} \middle| \psi \right\rangle \right], \quad (4)$$

where  $\hbar H$  is the quantum Hamiltonian of the system. In eq. (4)  $\psi$  is a vector in the Hilbert space  $\mathcal{H}$  for any moment of time  $t$ , and it belongs to the domain of the self-adjoint quasienergy operator  $K(t) = H - i\partial/\partial t$ . The variational principle for  $S$  applied on the entire Hilbert space  $\mathcal{H}$ , yields to the Schrödinger equation [57, 59].

By minimizing the action ( $\delta S = 0$ ), it can be shown that the Schrödinger equation is rigorously obtained from the variational principle. The natural symplectic structure induced by the transition probability between states for unitary transformations, achieved by the identification of the symplectic form with the imaginary part of the scalar product, enables approaching quantum mechanics issues through the formalism of the classical mechanics on (infinitely dimensional) symplectic manifolds (phase spaces), in particular Kähler manifolds.

We apply the variational principle to a manifold  $\widehat{\mathcal{M}}$  of test vectors, parametrized by the points of a finite  $2n$  dimensional phase space  $\mathcal{M}$ , with a Kähler manifold structure. In agreement with the Darboux theorem, the symplectic manifold  $\widehat{\mathcal{M}}$  admits canonical local coordinates and associated complex local coordinates. Generally the complex structure is not global, but local complex parametrization is preferred. In case of elementary quantum systems with dynamical symmetry groups which admit coherent states, the complex structure is global and  $\mathcal{M}$  represents a Kähler manifold.

#### 3.2. The Lagrange function. Hamilton equations of motion

We will consider  $z = (z_1, z_2, \dots, z_n) \in \mathcal{O}$  as a system of complex canonical local coordinates in  $\mathcal{M}$ , where  $\mathcal{O}$  is an open set from  $\mathbb{C}^n$ .  $\mathcal{M}$  is a manifold of dimension  $2n$ . The (global) symplectic structure and the (local) Kähler structure are induced on the variety of test vectors  $\widehat{\mathcal{M}}$ . We choose a family of vectors  $\psi(z) \in \widehat{\mathcal{M}}$  with  $z \in \mathcal{O}$ , holomorphic in  $z$ , such as  $\partial\psi(z)/\partial z_i^* = 0$ ,  $i = 1, \dots, n$ . The Lagrange function in the

complex parametrization can be expressed as

$$L(z, z^*) = \frac{i}{2 \langle \psi(z^*) | \psi(z) \rangle} \sum_{i=1}^n \left\{ \dot{z}_j \left\langle \psi(z^*) \left| \frac{\partial \psi(z)}{\partial z_i} \right. \right\rangle - \dot{z}_j^* \left\langle \frac{\partial \psi(z^*)}{\partial z_j} \left| \psi(z) \right. \right\rangle \right\} - \frac{\langle \psi(z^*) | H | \psi(z) \rangle}{\langle \psi(z^*) | \psi(z) \rangle}. \quad (5)$$

It is convenient to introduce the following notations [57]:

$$N(z, z^*) = \langle \psi(z^*) | \psi(z) \rangle, \quad H_{cl}(z, z^*) = \frac{\langle \psi(z^*) | H | \psi(z) \rangle}{\langle \psi(z^*) | \psi(z) \rangle}, \quad (6)$$

where  $H$  is the quantum Hamiltonian of the system, while  $H_{cl}$  stands for the classical Hamiltonian. Then the Lagrange function described by eq. (5) becomes

$$L(z, z^*) = \frac{i}{2} (\dot{z} \cdot \nabla_z - \dot{z}^* \cdot \nabla_{z^*}) \ln N(z, z^*) - H_{cl}(z, z^*), \quad (7)$$

where  $z \cdot \nabla_z = \sum_{i=1}^n z_i \partial_{z_i}$ . Hence the variation of the action is

$$\delta S = \int \left\{ i \sum_{j,k=1}^n \frac{\partial^2 \ln N}{\partial z_j \partial z_k^*} \dot{z}_j \delta z_k^* - i \sum_{j,k=1}^n \frac{\partial^2 \ln N}{\partial z_j^* \partial z_k} \dot{z}_j^* \delta z_k - \delta H_{cl} \right\}. \quad (8)$$

From the condition of extreme  $\delta S = 0$ , using independent variables, we obtain a system of equations such as :

$$i \sum_{j=1}^n \frac{\partial^2 \ln N}{\partial z_j^* \partial z_k} \dot{z}_j^* = -\frac{\partial H_{cl}}{\partial z_k}, \quad i \sum_{j=1}^n \frac{\partial^2 \ln N}{\partial z_j \partial z_k^*} \dot{z}_j = -\frac{\partial H_{cl}}{\partial z_k^*}. \quad (9)$$

We now introduce the matrix of the symplectic structure on  $\widehat{\mathcal{M}}$

$$\Omega = (\omega_{jk})_{1 \leq j, k \leq n}, \quad \omega_{jk} = \frac{\partial^2 \ln N}{\partial z_j \partial z_k^*}, \quad (10)$$

and Eqs. (9) change accordingly to

$$i \sum_{j=1}^n \omega_{kj} \dot{z}_j^* = -\frac{\partial H_{cl}}{\partial z_k}, \quad i \sum_{j=1}^n \omega_{jk} \dot{z}_j = \frac{\partial H_{cl}}{\partial z_k^*}, \quad (11)$$

where  $\omega_{jk}^* = \omega_{kj}$ . Hence we can ascertain that the matrix  $\Omega = \omega_{ij}$  is Hermitian. The Poisson brackets for the  $f, g \in C^\infty(\mathcal{M})$  functions, smooth on  $\mathcal{M}$ , can be introduced as:

$$\begin{aligned} \{f, g\} &= i \sum_{j,k=1}^n \left( \lambda_{jk} \frac{\partial f}{\partial z_j} \frac{\partial g}{\partial z_k^*} - \lambda_{kj}^* \frac{\partial g}{\partial z_j} \frac{\partial f}{\partial z_k^*} \right) = \\ &= \left( \frac{\partial f}{\partial z} \right)^t \Omega^{*-1} \frac{\partial g}{\partial z^*} + \left( \frac{\partial f}{\partial z} \right)^t \Omega^{-1} \frac{\partial g}{\partial z}, \end{aligned} \quad (12)$$

where  $\lambda_{jk} = -i(\Omega^*)^{-1}$ . Thus the variational principle for  $S$  applied on  $\widehat{\mathcal{M}}$  leads to the following equations of motion, which are classical [57]:

$$\frac{dz_j}{dt} = \{z, H_{cl}\}, \quad \frac{dz_j^*}{dt} = \{z^*, H_{cl}\}, \quad (13)$$



where

$$H_{cl}(z, z^*) = \frac{\langle \psi(z^*) | H | \psi(z) \rangle}{\langle \psi(z^*) | \psi(z) \rangle}. \quad (14)$$

This paper deals with the study of classical and semiclassical nonlinear dynamical systems. It focuses on similarities and differences found when comparing the dynamical behaviour of Hamiltonian systems described by classical theory in respect with those described by the quantum theory [82, 83]. An algorithm has resulted, through which an energy function is associated to the quantum Hamiltonian. This function represents a classical type Hamiltonian, whose values are precisely the expected values of the quantum Hamiltonian [12]. The energy function determines nonlinear equations of motion which can be approached using the theory of differential dynamical systems. It is suggested that this algorithm could be used in order to establish a correspondence between semiclassical and classical dynamics.

The phase space  $\mathcal{M}$  is a symplectic manifold described by eq. (10), with Poisson brackets determined by eq. (13). Eqs. (9) are the Hamilton equations which describe the Hamiltonian function  $H_{cl}$  on  $\mathcal{M}$ . Thus  $H_{cl}(z, z^*)$  is the expected value of the quantum Hamiltonian in the state represented by  $\psi(z) \in \widehat{\mathcal{M}}$ . Consequently  $H_{cl}$  is considered the classical Hamiltonian associated to the quantum Hamiltonian  $H$ . This association is usually called *dequantization* [84] and it represents a set of rules which turn quantum mechanics into classical. The solutions of the equations of motion for the classical Hamiltonian  $H_{cl}$  contain the same amount of spectral information as the solutions of the Schrödinger equation for the quantum Hamiltonian  $H$ , for many of the dynamical systems of interest. One of the conditions to be fulfilled is to choose  $\widehat{\mathcal{M}}$  as a manifold of coherent states.

The group of linear canonical transformations of a dynamical system with  $n$  degrees of freedom is the symplectic group  $\mathcal{Sp}(2n, \mathbb{R})$ . An electrically charged particle confined within an electromagnetic trap can be explicitly described using coherent states, for a subgroup  $\mathcal{G}$  of the symplectic group  $\mathcal{Sp}(6, \mathbb{R})$  [27, 29]. Symplectic transformations in  $\mathcal{Sp}(2n, \mathbb{R})$  leave invariant the canonical form of the classical Hamiltonian equations of motion [61, 67].

### 3.3. Symplectic coherent states. Algebraic models. Equations of motion

Further on we will introduce the coherent states built over the weight states of the discrete positive series of the symplectic group  $\mathcal{Sp}(2, \mathbb{R})$ , which is also a real Lie group [27, 55, 56, 85]. We will consider a unitary representation  $\mathcal{U}$  of the group  $\mathcal{Sp}(2, \mathbb{R})$  in the Hilbert space  $\mathcal{H}$ . We will denote by  $\mathcal{G}$  the group of unitary operators  $\mathcal{U}(g)$  with  $g \in \mathcal{Sp}(2, \mathbb{R})$  and by  $\mathfrak{g}$  the Lie algebra for this group (in fact, the  $SU(1, 1)$  Lie algebra). The algebra is determined by three generators  $K_0, K_1$ , and  $K_2$ . Further on we may define the ladder operators  $K_{\pm} = K_1 \pm iK_2$  so that the Lie algebra may be cast into canonical form [34] :

$$[K_0, K_{\pm}] = \pm K_{\pm}, \quad [K_-, K_+] = 2K_0. \quad (15)$$

The Lie algebra  $\mathfrak{sp}(2, \mathbb{R})$  consists of all the real linear combinations of the operators  $iK_0, iK_1$ , and  $iK_2$ . We will denote by  $\mathcal{U}_k$  a unitary irreducible subrepresentation of the  $\mathcal{U}$  representation in the Hilbert subspace  $\mathcal{H}_k$  of the  $\mathcal{H}$  space, where  $k$  stands for the Bargmann index [86]. The discrete series unitary representation of the Lie algebra considered are labelled by the eigenstates of the Casimir operator  $C$  [56]

$$C_2 = K_0^2 - K_1^2 - K_2^2, \quad (16)$$

with eigenvalues  $k(k-1)$  [74, 87, 88]. We will consider only irreducible unitary representations of the group  $\mathcal{Sp}(2, \mathbb{R})$ , corresponding to the discrete positive series  $\mathcal{D}^+(k)$  [34, 56, 74].

Coherent and squeezed states in Quantum Optics are concerned with the Positive Discrete Series  $\mathcal{D}^+(k)$ . The canonical orthonormal basis of the  $\mathcal{H}_k$  space consists of the  $|m, k\rangle$ ;  $m = 0, 1, \dots$ , vectors. For the representations of interest, the states  $|m, k\rangle$  diagonalize the compact operator  $K_0$ . The operators  $K_+$  and  $K_-$  are Hermitian conjugates of each other and act as raising and lowering operators of the quantum number  $m$  [34, 55, 71]:

$$\begin{aligned} K_+ |m, k\rangle &= [(m+1)(m+2k)]^{1/2} |m+1, k\rangle, \\ K_- |m, k\rangle &= [m(m+2k-1)]^{1/2} |m-1, k\rangle, \\ K_0 |m, k\rangle &= (m+k) |m, k\rangle. \end{aligned} \quad (17)$$

The coherent states for the symplectic group  $\mathcal{Sp}(2, \mathbb{R})$  are defined as [34]:

$$|z, m, k\rangle = U(z) |m, k\rangle, \quad (18)$$

Using the disentangling theorem for the  $SU(1, 1)$  Lie algebra [77, 78] the unitary operator  $U(z)$  can be expressed as

$$U(z) = \exp(zK_+) \exp(\beta K_0) \exp(-\bar{z}K_-), \quad (19)$$

where  $|z| < 1$  and  $\beta = \ln(1 - z\bar{z})$ . The  $|z, m, k\rangle$  states are called *symplectic coherent states*. The phase space  $\mathcal{M}$  whose points parametrize the coherent states is the unitary disk  $|z| < 1$ , endowed with the Lobachevski metrics  $ds^2 = 4(1 - z\bar{z})^{-2} dz d\bar{z}$ . For  $m = 0$  we infer the geometrical construction of Perelomov [14]. Eq. (18) remains valid for coherent states with  $m > 0$ , realized by applying the unitary operators  $U(z) \in \mathcal{G}$  on the nondominant weighting vectors  $|k, m\rangle$ ;  $m = 1, 2, \dots$ .

Using the Baker-Campbell-Hausdorff formula [67, 89] and eq. (18), we infer [55, 56, 90]

$$\begin{aligned} U^{-1}(z) K_0 U(z) &= (1 - z\bar{z})^{-1} [\bar{z}K_- + (1 + z\bar{z})K_0 + zK_+], \\ U^{-1}(z) K_+ U(z) &= (1 - z\bar{z})^{-1} [K_+ + 2\bar{z}K_0 + \bar{z}^2 K_-], \\ U^{-1}(z) K_- U(z) &= (1 - z\bar{z})^{-1} [K_- + 2zK_0 + z^2 K_+]. \end{aligned} \quad (20)$$

We will denote by  $\Omega_\varepsilon = K_0 + \varepsilon K_1$ , where  $\varepsilon = \pm 1$ . Then

$$U^{-1}(z) \Omega_\varepsilon U(z) = \frac{(1 + \varepsilon z)(1 + \varepsilon \bar{z})}{1 - z\bar{z}} E_\varepsilon, \quad (21)$$

$$E_\varepsilon = \frac{1}{2} (1 - z\bar{z})^{-1} [2(1+z)(1+\bar{z})K_0 + \varepsilon(1+\bar{z})^2 K_- + \varepsilon(1+z)^2 K_+] \quad (22)$$

From eqs. (20) - (22), we infer

$$\langle z, k, m | \Omega_\varepsilon^n | z, k, m \rangle = \left[ \frac{(1 + \varepsilon z)(1 + \varepsilon \bar{z})}{1 - z\bar{z}} \right]^n \langle k, m | E_\varepsilon^n | k, m \rangle . \quad (23)$$

Eq. (23) enables the explicit calculus of the Husimi function for every algebraic model with a dynamical group  $\mathcal{G}$ . If  $H$  is the Hamiltonian for such a model, expressed as a polynomial in the operators  $K_0, K_1$ , and  $K_2$ , we observe that the Hamiltonian function  $H_{cl}(z) = \langle z, k, m | H | z, k, m \rangle$  leads to the following equation of motion in the phase space  $\mathcal{M}$ :

$$\dot{z} = \{z, H_{cl}\} . \quad (24)$$

The brackets  $\{, \}$  stand for the Poisson brackets associated with the symplectic manifold  $\mathcal{M}$ , defined as [57, 59]

$$\{f, g\} = \frac{(1 - z\bar{z})^2}{2i(k + m)} \left( \frac{\partial f}{\partial z} \frac{\partial g}{\partial \bar{z}} - \frac{\partial f}{\partial \bar{z}} \frac{\partial g}{\partial z} \right) , \quad (25)$$

where the phase space classical observables  $f$  and  $g$  are smooth and real functions of  $\Re z$  and  $\Im z$ . When  $m = 0$ , from the TDVP applied to the coherent states  $|z, 0, k\rangle$  for the Hamiltonian  $H$  we infer Eqs. (24), which can also be expressed as

$$\dot{z} = \frac{(1 - z\bar{z})^2}{2ik} \frac{\partial H_{cl}}{\partial \bar{z}} . \quad (26)$$

We now introduce the complex variables  $\xi$  and  $\eta$  defined as

$$\xi = \frac{(1 + z)(1 + \bar{z})}{1 - z\bar{z}} , \quad \eta = \frac{(1 - z)(1 - \bar{z})}{1 - z\bar{z}} . \quad (27)$$

Then eqs. (26) become

$$\dot{\xi} = \frac{2}{ik} \frac{z - \bar{z}}{1 - z\bar{z}} \frac{\partial H_{cl}}{\partial \eta} , \quad \dot{\eta} = -\frac{2}{ik} \frac{z - \bar{z}}{1 - z\bar{z}} \frac{\partial H_{cl}}{\partial \xi} , \quad (28)$$

which are exactly the equations of motion in the phase space for the system we considered. The group of the linear canonical transformations of a dynamical system with  $n$  degrees of freedom, is the symplectic group  $Sp(2n, \mathbb{R})$  [81]. In case of dynamical symmetry groups, the Schrödinger equation solutions associated to linear Hamiltonians are given by coherent vectors multiplied by geometrical (Berry) phase factors [55]. The associated classical Hamiltonians result from the expected values of the quantum Hamiltonians on coherent symplectic states. Thus spectral information is coded into the phase portrait. The formalism presented here allows to explicitly construct bases and systems of symplectic coherent states for the study of trapped ion systems.

## 4. Semiclassical dynamics of an ion in combined traps with axial symmetry

### 4.1. Algebraic models for nonlinear axial traps

We have reviewed the properties of the coherent states and their exceptional importance for physics and especially for quantum optics. Coherent states for charged particles

confined in electrodynamic traps can be built using the group theory [91, 92]. We will further investigate the semiclassical dynamics of an ion trapped in a nonlinear electrodynamic trap with cylindrical symmetry, using the symplectic state approach and coherent state formalism developed in [14, 27, 29, 55], presented in Sections 3.2 and 3.3. The coherent state formalism is applied in order to study the semiclassical behaviour of trapped ions [27, 29, 55, 56]. We will introduce the Lie algebra generators of the axial symplectic group  $Sp(2, \mathbb{R})_a$  [27, 55]

$$K_{0,1a} = \frac{M\omega_a}{4\hbar} \left[ z^2 \pm \frac{p_z^2}{M^2\omega_a^2} \right], \quad K_{2a} = \frac{i}{4\hbar} \left[ 2z \frac{\partial}{\partial z} + 1 \right], \quad (29)$$

and the Lie algebra generators of the radial symplectic group  $Sp(2, \mathbb{R})_r$  for a fixed eigenvalue of the orbital angular momentum  $\hbar l$

$$K_{0,1r} = \pm \frac{1}{2\hbar\omega_r} \left[ \frac{1}{2M} p_\rho^2 \pm \frac{M\omega_r^2}{2} \rho^2 + \frac{\hbar^2}{2M} \left( l^2 - \frac{1}{4} \right) \frac{1}{\rho^2} \right], \quad (30)$$

$$K_{2r} = \frac{i}{4\hbar} \left[ 2\rho \frac{\partial}{\partial \rho} + 1 \right].$$

We have denoted by  $\omega_a/2\pi$  the axial frequency and by  $\omega_r/2\pi$  the radial frequency respectively, of the quadrupole trap potential. The  $K_{0j}, K_{1j}$  and  $K_{2j} = i[K_{1j}, K_{0j}], j = a, r$  operators satisfy the commutation relations for the Lie algebra of the symplectic group  $Sp(2, \mathbb{R})$

$$[K_{0j}, K_{1j}] = iK_{2j}, \quad [K_{2j}, K_{0j}] = iK_{1j}, \quad [K_{2j}, K_{1j}] = iK_{0j}. \quad (31)$$

Then the quantum Hamiltonian of a particle with electrical charge  $Q$ , mass  $M$  and orbital angular momentum  $\hbar l$ , located in the quadrupole trap with octopole anharmonicity, can be expressed as [90]

$$H_l = -\frac{4Q\hbar}{M\omega_a} A(t) (K_{0a} + K_{1a}) + \frac{\hbar}{\omega_r} \left( \frac{\omega_c^2}{4} + \frac{2Q}{M} A(t) \right) (K_{0r} + K_{1r}) - \frac{\omega_c}{2} \hbar l + \hbar\omega_a (K_{0a} - K_{1a}) + \hbar\omega_r (K_{0r} - K_{1r}) + c_2 A(t) H_4(\rho, z), \quad (32)$$

where  $\omega_c$  stands for the cyclotronic frequency and  $H_4$  is a harmonic polynomial of degree 2 homogeneous in the variables  $z^2$  and  $\rho^2 = x^2 + y^2$ . These variables can be expressed as a function of the generators

$$z^2 = \frac{4\hbar}{M\omega_a} (K_{0a} + K_{1a}), \quad \rho^2 = \frac{4\hbar}{M\omega_r} (K_{0r} + K_{1r}). \quad (33)$$

The coupling constant  $c_2$  and the time dependent function  $A(t)$  are characteristic to the type of trap and will be explained later.

Eq. (32) results from the general expression of the Hamiltonian associated to a particle which undergoes the influence of an electromagnetic field, characterized by an electrical potential  $\Phi$  and a magnetic induction  $\vec{B}$  [19, 27, 29, 85]:

$$H = \frac{1}{2M} \left[ \vec{p} - \frac{1}{2} Q\vec{B} \times \vec{r} \right]^2 + Q\Phi. \quad (34)$$

The momentum operator for the particle is  $\vec{p} = -i\hbar\nabla$ , while the magnetic field is considered to be axial:  $\vec{B} = (0, 0, B_0)$  and  $\omega_c = QB_0/M$ . We can introduce the (axial) angular momentum operator on the  $z$  axis, defined as  $L_z = xp_y - yp_x$ . Then Eq. (34) becomes

$$H = \frac{1}{2M} (p_x^2 + p_y^2 + p_z^2) + \frac{1}{8M} Q^2 B_0^2 \rho^2 - \frac{QB_0}{2M} L_z + Q\Phi . \quad (35)$$

Because the axial angular momentum operator  $L_z$  commutes both with the symplectic groups generators as well as with the Hamiltonian  $H$ , the study of the quantum system can be restricted to a subspace of the Hilbert space for which  $L_z = \hbar l I$ , where  $l$  is the orbital quantum number. The Hamiltonian reduced to this subspace can be expressed as

$$H_l = \frac{1}{2M} (p_x^2 + p_y^2 + p_z^2) + \frac{1}{8M} Q^2 B_0^2 \rho^2 - \frac{QB_0}{2M} \hbar l + Q\Phi . \quad (36)$$

Choosing a system of cylindrical coordinates  $\rho$  and  $\theta$ , the expressions for the radial coordinates are  $x = \rho \cos \theta$  and  $y = \rho \sin \theta$ . It follows that

$$p_x^2 + p_y^2 = -\hbar^2 \left( \frac{\partial^2}{\partial \rho^2} + \frac{1}{\rho^2} \frac{\partial^2}{\partial \theta^2} + \frac{1}{\rho} \frac{\partial}{\partial \rho} \right) , \quad L_z = -i\hbar \frac{\partial}{\partial \theta} . \quad (37)$$

We choose  $\Psi = e^{il\theta} \chi$  as a solution of the Schrödinger equation, where  $\chi$  depends only on  $\rho$  and  $z$ . Then  $L_z \Psi = \hbar l \Psi$  and  $\chi$  is a solution of the Schrödinger equation for the Hamiltonian

$$H_l = -\frac{\hbar^2}{2M} \left( \frac{\partial^2}{\partial \rho^2} - \frac{l^2}{\rho^2} + \frac{1}{\rho} \frac{\partial}{\partial \rho} \right) - \frac{\hbar^2}{2M} \frac{\partial^2}{\partial z^2} + \frac{M\omega_c^2}{8} \rho^2 - \frac{\omega_c}{2} \hbar l + Q\Phi , \quad (38)$$

which results from Eqs. (36) and (37).

We will now choose a potential with axial symmetry, such as

$$\Phi(\vec{r}, t) = A(t) g(\rho, z) , \quad (39)$$

where  $A(t)$  is a time-periodical function of period  $T = 2\pi/\Omega$ , while  $g$  is a function of  $\rho^2$  and  $z^2$  which satisfies

$$g(\rho, z) = \sum_{k \geq 1} c_k H_{2k}(\rho, z) . \quad (40)$$

The  $H_{2k}$  polynomials are harmonic polynomials of degree  $k$  in  $\rho^2$  and  $z^2$ . The potential described by Eq. (39) is characteristic for a trap with axial symmetry and with symmetry in respect to the radial plane  $xOy$ . For a Penning trap  $A$  is constant in time, but for most of the radiofrequency traps we choose  $A(t) = U_0 + V_0 \cos \Omega t$ . In case of a harmonic potential ( $c_k = 0$  for  $k > 1$ ) we have

$$g(\rho, z) = \frac{1}{r_0^2 + 2z_0^2} (\rho^2 - 2z^2) , \quad c_2 = -\frac{1}{r_0^2 + 2z_0^2} , \quad (41)$$

where  $r_0$  and  $z_0$  are the semiaxes of the combined quadrupole trap we have considered. We remind that a combined trap consists of a Penning trap and a superimposed Paul trap. The particular case of the ideal Paul trap is obtained for  $\vec{B} = 0$ . The quadrupole potential is produced by hyperbolic electrodes. Real traps are different from ideal ones.

Due to mechanical imperfections (holes drilled in the endcap electrodes or in the ring electrode, the latter causing a radial asymmetry of the potential), the trap potential is not a pure quadrupole potential. The potential is then expanded in a power series and higher order terms have to be considered. Due to the trap symmetry we have chosen, the odd terms of higher order from the series expansion of the potential vanish and we are left only with the even terms. In case of a quadrupole trap with octopole anharmonicity, the electric potential can be expressed as

$$g(\rho, z) = c_1 H_2(\rho, z) + c_2 H_4(\rho, z) , \quad (42)$$

$$H_2(\rho, z) = 2z^2 - \rho^2 , \quad H_4(\rho, z) = 8z^4 - 24z^2\rho^2 + 3\rho^4 . \quad (43)$$

where  $H_2$  is the pure quadrupole term and  $H_4$  is the octopole term. Under such case, the Hamiltonian  $H_l$  is given by Eq. (32). The next anharmonical contribution is given by the polynomial

$$H_6 = 16z^6 - 120z^4\rho^2 + 90z^2\rho^4 - 5\rho^6 . \quad (44)$$

By denoting

$$K_r = \frac{M\omega_c^2}{4} - 2Qc_2A(t) , \quad K_a = 4Qc_2A(t) ,$$

the Hamiltonian given by Eq. (38) can be expressed as

$$H_l = -\frac{\hbar^2}{2M} \left( \frac{\partial^2}{\partial \rho^2} - \frac{l^2}{\rho^2} + \frac{1}{\rho} \frac{\partial}{\partial \rho} \right) - \frac{\hbar^2}{2M} \frac{\partial^2}{\partial z^2} - \frac{\omega_c}{2} \hbar l + \frac{K_r}{2} \rho^2 + \frac{K_a}{2} z^2 + QA(t) P(\rho^2, z^2) , \quad (45)$$

where the anharmonical part is defined as

$$P(\rho^2, z^2) = \sum_{k \geq 2} c_k H_{2k}(\rho, z) . \quad (46)$$

In the following we will study the Schrödinger equation

$$i\hbar \frac{\partial \chi}{\partial t} = H_l \chi ,$$

where  $H_l$  is given by Eq. (45), with particularizations for combined quadrupole and octopole traps. In agreement with Eqs. (32), (33) and (45), The Hamiltonian  $H_l$  describes an algebraic model when  $P(\rho^2, z^2)$  is a polynomial function. This model is linear for quadrupole traps ( $P$  is a linear combination between  $\rho^2$  and  $z^2$ ) [90].

#### 4.2. Dynamical symmetries for an ion in an axial trap

The algebraic model described by the Hamiltonian  $H_l$  can be characterized by the dynamical symmetry group  $\mathcal{G} = \mathcal{G}_a \otimes \mathcal{G}_r$ , realized as a direct product between the axial symplectic group  $\mathcal{G}_a = \mathcal{Sp}(2, \mathbb{R})_a$  and the radial symplectic group  $\mathcal{G}_r = \mathcal{Sp}(2, \mathbb{R})_r$  [56, 93].

From Eqs. (30) we obtain the commutation relations

$$[K_{0a}, K_{1a}] = iK_{2a} , \quad [K_{2a}, K_{0a}] = iK_{1a} , \quad [K_{1a}, K_{2a}] = iK_{0a} , \quad (47)$$

for the Lie algebra  $\mathfrak{g}_a$  of the group  $\mathcal{G}_a$ . The Casimir operator of the Lie algebra  $\mathfrak{g}_a$  determines the Bargmann indexes  $k$ , and it can be expressed as [55, 56, 71]

$$C_{2a} = K_{0a}^2 - K_{1a}^2 - K_{2a}^2 = -\frac{3}{16}I = k(k-1)I , \quad (48)$$

where  $I$  is the unitary operator. From Eq. (48) we infer the values of the two Bargmann indexes which characterize the axial motion

$$k_{a+} = \frac{1}{4} , \quad k_{a-} = \frac{3}{4} . \quad (49)$$

From Eqs. (30) we obtain the commutation relations

$$[K_{0r}, K_{1r}] = iK_{2r} , \quad [K_{2r}, K_{0r}] = iK_{1r} , \quad [K_{1r}, K_{2r}] = iK_{0r} , \quad (50)$$

for the Lie algebra  $\mathfrak{g}_r$  of the group  $\mathcal{G}_r$ . The Casimir operator of the Lie algebra  $\mathfrak{g}_r$  is [34, 56, 90]

$$C_{2r} = K_{0r}^2 - K_{1r}^2 - K_{2r}^2 = \frac{l^2 - 1}{4} I = k(k-1)I . \quad (51)$$

From Eq. (51) we infer the Bargmann index  $k_r = (l+1)/2$ , where  $l$  represents the quantum orbital number. Eq. (45) can be now expressed as

$$\begin{aligned} H_l &= \hbar\omega_r (K_{0r} - K_{1r}) + 2\hbar\omega_a (K_{0a} - K_{1a}) - \frac{\omega_c}{2}\hbar l \\ &+ \frac{K_r}{2} \frac{2\hbar}{M\omega_r} (K_{0r} + K_{1r}) + \frac{K_a}{2} \frac{2\hbar}{M\omega_a} (K_{0a} + K_{1a}) + QA(t)P(\rho^2, z^2) . \end{aligned} \quad (52)$$

Consequently, the study of the Hamiltonian for an ion confined in a quadrupole trap ( $P = 0$ ) has been restricted to the study of a linear model for the dynamic group  $\mathcal{G}$ , for which the irreducible unitary representations are characterized by the Bargmann indexes  $k_a$  and  $k_r$ , fixed [55]. The solutions of the Schrödinger equation for this elementary quantum system will result explicitly by using the coherent state formalism for the group  $\mathcal{G}$ . This formalism will be also used for algebraic models which describe nonlinear traps (with  $P \neq 0$ ).

It can be shown that symplectic coherent states are realized in the trapped ion dynamics and a classical Hamiltonian (the Husimi or the energy function) can be associated to the quantum Hamiltonian. The Hamiltonian function leads to equations of motion in the classical Lobachevski phase space.

### 4.3. Symplectic coherent states representation

According to paragraph 4.2, the Bargmann indexes for the axial motion are given by  $k_- = \frac{1}{4}$  and  $k_+ = \frac{3}{4}$ , while in case of the radial motion the expression is  $k_l = (1+l)/2$ , where  $l$  stands for the orbital quantum number. The canonical orthonormal basis of the Hilbert space for an irreducible unitary representation of the group  $\mathcal{G}_j$ , of Bargmann

index  $k_j$ , with  $j = a, r$ , consists of the vectors  $\phi_{jm}$ ,  $m = 0, 1, \dots$  and it is characterized by the equations

$$K_{0j}\phi_{jm} = (k_j + m)\phi_{jm}, \quad K_{-j}\phi_{jj} = 0. \quad (53)$$

We can introduce the coherent symplectic vectors  $\psi_{jm}(z_j)$ , defined as

$$\psi_{jm}(z_j) = U_j(z) \phi_{jm}, \quad (54)$$

$$U_j(z_j) = \exp(z_j K_{+j}) \exp(\beta_j K_{0j}) \exp(-\bar{z}_j K_{-j}), \quad (55)$$

where  $U_j(z_j)$  are unitary operators of the representation,  $\beta_j = \ln(1 - z_j \bar{z}_j)$ , and  $z_j$  is a complex variable from the unit disk  $|z_j| < 1$ . The phase space  $\mathcal{M}$  associated to an ion confined within an axial symmetry trap represents the product of the axial and radial unit disks, realized as a bound domain in  $\mathbb{C}^2$ , made out of all points  $(z_a, z_r)$  with  $|z_a| < 1$  and  $|z_r| < 1$ . The coherent states for the dynamical group  $\mathcal{G}$ , parametrized with points from  $\mathcal{M}$ , can be expressed as

$$\Phi_{m_a m_r}(z_a, z_r) = \psi_{a m_a}(z_a) \psi_{r m_r}(z_r). \quad (56)$$

In case of quadrupole traps, the symplectic coherent states  $\Phi_{m_a m_r}(z_a, z_r)$  multiplied by Berry phase factors are solutions of the Schrödinger equation [55].

The energy function associated to the Hamiltonian (52) represents a classical Hamiltonian  $H_{cl}$  on  $\mathcal{M}$ , whose values are exactly the expected values of the Hamiltonian  $H_l$  on coherent states  $\Phi_{m_a m_r}(z_a, z_r)$ , such as

$$\begin{aligned} H_{cl} = & \hbar\omega_r (k_r + m_r) \frac{(1 - z_r)(1 - \bar{z}_r)}{1 - z_r \bar{z}_r} + 2\hbar\omega_a (k_a + m_a) \frac{(1 - z_a)(1 - \bar{z}_a)}{1 - z_a \bar{z}_a} \\ & + \frac{2\hbar K_r}{M\omega_r} (k_r + m_r) \frac{(1 + z_r)(1 + \bar{z}_r)}{1 - z_r \bar{z}_r} + \frac{2\hbar K_a}{M\omega_a} (k_a + m_a) \frac{(1 + z_a)(1 + \bar{z}_a)}{1 - z_a \bar{z}_a} \\ & - \frac{\omega_c}{2} \hbar l + H_{anarm}, \end{aligned} \quad (57)$$

cu

$$H_{anarm} = QA(t) \langle P(\rho^2, z^2) \rangle = QA(t) \sum_{k \geq 1} c_k \langle H_{2k}(\rho, z) \rangle. \quad (58)$$

We have denoted by  $\langle X \rangle$  the expected value of the operator  $X$  in the coherent state  $\Phi_{m_a m_r}(z_a, z_r)$ . In particular we obtain

$$\langle H_4 \rangle = 8S_{2a} - 24S_{1r}S_{2r} + 3S_{2r}, \quad (59)$$

$$\langle H_6 \rangle = 16S_{3a} - 120S_{2a}S_{1r} + 90S_{1a}S_{2r} - 5S_{3r}. \quad (60)$$

where

$$S_{jr} = S_j(z_r, k_r, m_r), \quad S_{ja} = S_j(z_a, k_a, m_a), \quad 1 \leq j \leq 3,$$

with

$$S_j(z, k, m) = \left[ \frac{(1+z)(1+\bar{z})}{1-z\bar{z}} \right]^j Q_j(k, m), \quad (61)$$



and

$$Q_1(k, m) = 2(k + m) \quad (62)$$

$$Q_2(k, m) = 2k(2k + 1) + 12km + 6m^2 \quad (63)$$

$$Q_3(k, m) = 4k(k + 1)(2k + 1) + 4mk(5 + 12k) + 4m^2(15k + 1) + 20m^3 \quad (64)$$

The values of the indexes are :

$$m_a, m_r = 0, 1, \dots ; k_a = \frac{1}{4}, \frac{3}{4} ; k_r = \frac{l+1}{2} .$$

We will introduce the complex variables  $\xi_j$  and  $\eta_j$ ,  $j = a, r$ , defined as

$$\xi_j = \frac{(1 + z_j)(1 + \bar{z}_j)}{1 - z_j\bar{z}_j} , \quad \eta_j = \frac{(1 - z_j)(1 - \bar{z}_j)}{1 - z_j\bar{z}_j} . \quad (65)$$

Then the classical Hamiltonian (the Husimi function) for an octupole trap in case of the pseudopotential approximation can be expressed as

$$\begin{aligned} H_{cl} = & A_r\eta_r + A_a\eta_a + B_r\xi_r + B_a\xi_a + (C_{20}\xi_r^2 + C_{11}\xi_r\xi_a + C_{02}\xi_a^2) \\ & + (D_{30}\xi_r^3 + D_{21}\xi_r^2\xi_a + D_{12}\xi_r\xi_a^2 + D_{03}\xi_a^3) - \frac{\omega_c}{2}\hbar l. \end{aligned} \quad (66)$$

If  $P$  is a polynomial of  $\rho^2$  and  $z^2$ , then  $H_{cl}$  is a polynomial of  $\xi_a$  and  $\xi_r$ . In order to find the minimum points of the Husimi function we have to solve the equations

$$\frac{\partial H_{cl}}{\partial \xi_a} = 0 , \quad \frac{\partial H_{cl}}{\partial \xi_r} = 0 , \quad \frac{\partial H_{cl}}{\partial \eta_a} = 0 , \quad \frac{\partial H_{cl}}{\partial \eta_r} = 0 . \quad (67)$$

It can be observed that the Hamiltonian function  $H_{cl} = \langle z, k, m | H | z, k, m \rangle$  determines the following equation of motion in the classical Lobachevski phase space  $|z| < 1$  :

$$\dot{z} = \{z, H_{cl}\} , \quad (68)$$

where  $\{ , \}$  stands for the generalized Poisson bracket, defined in Eq. (25) [57]. After applying the TDVP to the coherent states  $|z, 0, k\rangle$  for the Hamiltonian  $H$  we infer Eqs.

$$\{z, H_{cl}\} = \frac{(1 - z\bar{z})^2}{2ik} \frac{\partial H_{cl}}{\partial \bar{z}} \quad (69)$$

which represents a classical type equation of motion. If  $P$  given by Eq. (46) is a polynomial in  $\rho^2$  and  $z^2$ , then  $H_{cl}$  is a polynomial in  $\xi_a$  and  $\xi_r$ .

The results obtained here can be extended to a system of  $N$  particles (ions), confined in a quadrupole electromagnetic trap with cylindrical symmetry [56, 27, 29]. As shown in these references, the Hamiltonian of the center of mass (CM) is similar to the Hamiltonian for one particle  $H$ , given by Eq. (34). Then the quasienergy states and the coherent states are exactly those for the  $H$  Hamiltonian, where we have to substitute  $M$  the mass of one particle with  $NM$ . In case when the interaction potential is translation invariant and homogeneous of degree  $-2$ , we obtain soluble models (e.g., for Calogero type potentials). These models enable to explicitly obtain bases and systems of symplectic coherent states, in order to investigate ordered systems made of trapped ions.

## 5. Conclusions

The widest class of quantum models which describe both analytically and numerically the energy spectra and the solutions of the Schrödinger equation, is made of elementary quantum systems (in the Wigner sense). An elementary quantum system is described by an irreducible unitary representation  $\mathcal{U}$  of a dynamical group  $\mathcal{G}$  on a Hilbert space  $\mathcal{H}$ . The space of states is the quantum phase space  $\mathcal{P}(\mathcal{H})$ , with the symplectic structure induced by the transition probability. It is assumed that the representation  $\mathcal{U}$  admits coherent states. Then, coherent states manifolds are orbits of the action of the dynamical group on the space of states. The quantum Hamiltonian is a polynomial in the generators of the Lie algebra  $\mathfrak{g}$  of the group  $\mathcal{G}$ . This property is specific to dynamical groups considered as spectrum generating groups. The energy (Husimi) function associated to the quantum Hamiltonian  $H$  is a classical type Hamiltonian, whose values are precisely the expected values of the quantum Hamiltonian on coherent states.

Thus the quantum dynamical system is considered as a Hamiltonian system over the phase space of quantum states, while the corresponding classical system is described by the energy (Husimi) function over the phase space  $\mathcal{M}$ , whose points parametrize the coherent states. The symplectic structure of the classical phase space and the Hamilton equations of motion are explicitly obtained using the variational principle applied on coherent states and from the theory of group representation.

This paper deals with the study of classical and semiclassical nonlinear dynamical systems. It focuses on similarities and differences found when comparing the dynamical behaviour of Hamiltonian systems described by classical theory in respect with those described by the quantum theory [82]. An algorithm has resulted, through which an energy function is associated to the quantum Hamiltonian. This function represents a classical type Hamiltonian, whose values are precisely the expected values of the quantum Hamiltonian. The energy function determines nonlinear equations of motion which can be approached using the theory of differential dynamical systems. It is suggested that this algorithm can be used to establish a correspondence between semiclassical and classical dynamics.

Semiclassical dynamics of trapped ions has been investigated by introducing the coherent state orbits as sub-manifolds of the quantum states' space with a Kähler structure induced by the transition probability. In case of dynamical symmetry groups, the solutions of the Schrödinger equation associated to linear Hamiltonians (in the infinitesimal generators of a dynamical symmetry group) are given by coherent vectors multiplied by geometric (Berry) phase factors for a confined ion or for the center of mass (CM) of a system of identical ions. Thus we obtain an energy spectrum for the time independent Hamiltonians (the case of Penning type traps) or a quasienergy spectrum for time periodical Hamiltonians (in case of dynamical Paul traps). The coherent states are parametrized by the solutions of the classical equations of motion.

These results have been extended to the case of an ion confined in a quadrupole electromagnetic trap with anharmonicities (a situation according to reality), in order

to study semiclassical dynamics associated to ions. Identification of equilibrium configurations is of interest for quantum information processing. We have obtained the explicit expression of the quantum Hamiltonian associated to a charged particle, located in an nonlinear electromagnetic trap (with anharmonicities), as a function of the Lie algebra generators for the radial and axial symplectic groups. The Schrödinger equation solution was found for the Hamiltonian we considered. An analytical potential with cylindrical symmetry was chosen. The Hamiltonian was particularized to the case of combined, quadrupole and octopole traps. In case of the pseudopotential approximation, the minimum points of the dequantified Hamiltonian define the equilibrium configurations for trapped ions, which enable implementing and scaling of quantum logic for larger number of ions.

Although the Schrödinger equation is nonlinear, the Hamiltonian (Husimi) function generally determines nonlinear equations of motion which can be investigated using the theory of differential dynamical systems. This theory enables qualitative global investigation of Hamilton families, depending on various control parameters. In particular it allows to describe classical chaos using Morse theory, bifurcation theory and catastrophe theory. Thus quantum chaos is described using the methods of study for the deterministic classical chaos. This description is possible through implicit codification in the Husimi function of the spectral properties of the Schrödinger operator. Dequantization by means of coherent states enables to achieve exact connexions between symmetrical quantum and classical dynamical systems. For an ion confined within a quadrupole trap, the requantification corresponds to a geometrical quantification.

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