STUDY OF QUASICLASSICAL DYNAMICS OF TRAPPED IONS USING THE COHERENT STATE FORMALISM AND ASSOCIATED ALGEBRAIC GROUPS

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Abstract. The time dependent variational principle (TDVP) has been applied on coherent state orbits and the Hamilton equations of motion on Kähler (symplectic) manifolds result. The classical Hamilton functions associated to the system are realized as the expected values of the quantum Hamiltonian on symplectic coherent states. The formalism applies to Hamilton functions that are nonlinear in the infinitesimal generators of a dynamical symmetry group (in case of 3D ion traps). Using symplectic coherent states, the explicit classical equations of motion on the unit disk have been obtained for any algebraic model that admits the dynamical group $Sp(2,\mathbb{R})$. The corresponding quasienergy states are explicitly realized as coherent states parameterized by the stable solutions of the corresponding classical equations of motion. The explicit expression of the quantum and classical Hamilton functions, particularized for combined (Paul and Penning) and ideal Paul traps, are obtained for the first time, taking into consideration the effect of trap electric potential nonlinearities. We also obtain the explicit equations of motion for a combined octupole trap, which represents an original result. A dequantization algorithm results.

Key words: Trapped ion; symplectic coherent states; dynamical symmetry group; nonlinear electromagnetic trap; quasienergy state.

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1. INTRODUCTION

The quantum time-dependent harmonic oscillator (TDHO) is used to describe the dynamics of many physical systems [1–5]. The paper uses recent results from the coherent state formalism developed in [4, 9], and applies it in particular to the study of quantum dynamics of ions confined in 3D ion traps.

The time-dependent Schrödinger equation for harmonic oscillators can be solved when the Hamiltonian is a linear combination of the generators that span the Lie algebra associated to the SU(1,1) group [6, 7], using the so-called *Peremolov's generalized coherent states* [8, 9]. Quantum dynamics in a 3D RF (Paul) ion trap was characterized by means of coherent states, using time-dependent quantum oscillator equations obtained by separating the axial and radial motion from the Schrödinger

equation [10]. In agreement with Ref. [7], the coherent state approach leads to quantum solutions that are explicitly constructed as functions of the classical trajectories on the phase space. Time-dependent Gaussian-like wave packets generalizing odd coherent states of the harmonic oscillator and excitation number eigenstates are constructed in Ref. [11], to describe the relative one-dimensional motion of two ions in a trap. The high repulsive centrifugal potential is shown to approximate, up to a certain extent, the real Coulomb repulsion between two trapped ions. The results obtained in [7, 10] are extended in Ref. [12], with an aim to characterize collective dynamics for systems of ions confined in quadrupole 3D ion traps that exhibit axial symmetry. The exact wavefunctions for a particle trapped by oscillating fields are obtained in terms of Mathieu functions in [13], and quantum solutions of a generalized inverted or repulsive harmonic oscillator with arbitrary time-dependent mass and frequency are obtained in Ref. [14], using linear invariants and the dynamical or quantum invariant method. In Ref. [15] the authors provide a method of finding a set of generators that form a closed Lie algebra, in order to describe a general quantum quadratic Hamiltonian, implicitly the evolution operator (propagator). The Lie algebra is then used to characterize the Hamiltonian of a charged particle in time-dependent electromagnetic fields, by identifying the similarities between the terms of these two Hamiltonians. Our approach within the paper consists in applying the results described above, and especially the coherent state formalism and the Hamilton formalism, to particular systems of ions confined in nonlinear (anharmonic) 3D ion traps (both combined and RF traps), with an aim to characterize the associated quasiclassical dynamics.

Superpositions of quantum arbitrary states for an ion trapped within a harmonic potential well are investigated in Ref. [9, 16], while also testing quantum theory limits along the mysterious frontier which separates quantum and classic worlds [17–20].

We apply and develop the coherent state formalism introduced in [6–8, 10, 12], and further developed in [4, 9], and the time dependent variational principle (TDVP) [21–23], with an aim to characterize quasiclassical behaviour of trapped ions and bring new evidence. We investigate the bosonic realization of the Lie algebra for the SU(1,1) group and (generalized) coherent states in the Fock space [24–26], particularized to the case of an ion confined within quadrupole and octupole combined traps. We propose a dequantization algorithm by which the classical Hamilton function is achieved exactly as the quantum Hamilton function on coherent states. It is for the first time that we give the explicit expression of the quantum Hamilton function associated to an ion confined in nonlinear 3D ion traps, and show that it describes an algebraic model when the anharmonic part is a polynomial. The model is linear only for quadrupole traps. The method suggested in [10, 27] is particularized for both nonlinear combined and ideal Paul traps, which represents an original, new result. The classical Hamilton equations of motion are obtained in case of octupole traps, a

result which we report for the first time. We also show that, when the pseudopotential approximation is valid, the minimum points of the classical Hamiltonian define equilibrium configurations for trapped ions.

The paper is organized as follows: In Section 3.2 the expression of the quantum Hamiltonian is obtained for quadrupole anharmonic traps that exhibit cylindrical symmetry. An algorithm is suggested which enables explicit calculus of the Hamilton function for every algebraic model with an associated dynamical group. Section 3.3 presents the solutions of the Schrödinger equation and the quasienergy spectrum for the model we suggest. We test our model in Section 4, where it is applied for quadrupole and octupole traps. The explicit expressions for the classical Hamilton functions are obtained in case of such particular traps, as well as the classical equations of motion, which represent highly original results. A discussion is performed in Section 5.

2. COHERENT STATES AND DYNAMICAL SYMMETRY GROUPS FOR 3D ION TRAPS

2.1. ELEMENTARY QUANTUM SYSTEMS AND ASSOCIATED COHERENT STATES

We recall some definitions from the geometry of coherent states [8, 16, 26]. We denote by $P(\mathcal{H})$ the quantum state space, where $\mathcal{H}$ is a separable complex Hilbert space of the state vectors (quantum states). To every non-zero vector $\psi \in \mathcal{H}$ we associate the $\widehat{\psi}$ state, realized as the set of all vectors $\gamma\psi$, where γ is complex. We consider an unitary irreducible representation (UIR) $\mathcal{U}$ of the Lie group $\mathcal{G}$ on $\mathcal{H}$. This representation induces an action $\hat{\mathcal{U}}$ of the $\mathcal{G}$ group on $P(\mathcal{H})$, defined as $\hat{\mathcal{U}}(g)\hat{\psi} = \widehat{\mathcal{U}(g)\psi}$, for any $g \in \mathcal{G}$ and any non-zero vector $\psi \in \mathcal{H}$. The orbit $\mathcal{O}_{\hat{\psi}}$ consists of all the states $\hat{\mathcal{U}}(g)\hat{\psi}$ for $g \in \mathcal{G}$. The elements of the orbit $\mathcal{O}_{\hat{\psi}}$ are called coherent states. We assume that the orbit $\mathcal{O}_{\hat{\psi}}$ is a sub-manifold of the space $\mathcal{P}(\mathcal{H})$, endowed with a Kähler space structure induced by the transition probability. Coherent state Kähler orbits are obtained for Heisenberg groups, compact groups and semisimple groups, whose representations belong to the holomorphic discrete series. Thus, a family of coherent states enables describing of the system by means of the associated classical trajectories.

2.2. HAMILTON EQUATIONS AND DEQUANTIZATION ALGORITHM

A canonical Hamiltonian formulation for the general time-dependent variational principle associated with the Schrödinger equation is discussed in [23, 28]. Since the Time-Dependent Hartree-Fock (TDHF) phase space is the classical correspondent of the quantum space of states (*i.e.*, a coherent state representation of the boson-mapped fermion space of states), classical information obtained from the

TDHF trajectories supplies us with relevant data on the structure change which occurs in the quantum space of states [29]. We consider the action integral [22]

$$S = \int \frac{1}{\langle\psi|\psi\rangle}\left[\langle\psi|H|\psi\rangle - \Im m\left\langle\frac{\partial\psi}{\partial t}\middle|\psi\right\rangle\right], \tag{1}$$

where $\hbar H$ is the quantum Hamiltonian. In eq. (1) ψ is a vector in the Hilbert space $\mathcal{H}$ that belongs to the domain of the self-adjoint quasienergy operator $K(t) = H - i\partial/\partial t$ [3]. By minimizing the action ($\delta S = 0$), it can be shown that the Schrödinger equation is rigurously obtained from the variational principle [22]. The natural symplectic structure induced by the transition probability between states for unitary transformations, 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 $\mathcal{M}$. In case of elementary quantum systems with dynamical symmetry groups which admit coherent states, the complex structure is global and $\hat{\mathcal{M}}$ represents a Kähler manifold. We consider $z = (z_1, z_2, \ldots, z_n) \in \mathcal{O}$ to be a system of complex canonical local coordinates in $\mathcal{M}$, where $\mathcal{O}$ is an open set from $\mathbb{C}^n$, 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 $\partial\psi(z)/\partial z_i^* = 0$, $i = 1, \ldots, n$. We denote [22]:

$$N(z, z^*) = \langle\psi(z^*)|\psi(z)\rangle \ , \ H_{cl}(z, z^*) = \frac{\langle\psi(z^*)|H|\psi(z)\rangle}{\langle\psi(z^*)|\psi(z)\rangle} \ , \tag{2}$$

where H is the quantum Hamiltonian of the system, and H_{cl} stands for the classical Hamiltonian. The Lagrange function in the complex parametrization can be expressed as

$$L(z,\ z^*) = \frac{i}{2}\left(\dot{z}\nabla_z - \dot{z}^*\nabla_{z^*}\right)\ln N(z, z^*) - H_{cl}(z, z^*) \ , \tag{3}$$

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

$$\delta S = \int \left\{ i \sum_{j,k=1}^{n} \frac{\partial^2 \ln N}{\partial z_j \partial z_k^*}\ \dot{z}_j \delta z_k^* - i \sum_{j,k=1}^{n} \frac{\partial^2 \ln N}{\partial z_j^* \partial z_k}\ \dot{z}_j^* \delta z_k - \delta H_{cl} \right\}. \tag{4}$$

Further on we introduce the matrix of the symplectic structure on $\widehat{\mathcal{M}}$ as

$$\Omega = (\omega_{jk})_{1 \le j,k \le n} \ , \ \omega_{jk} = \frac{\partial^2 \ln N}{\partial z_j \partial z_k^*} \ , \tag{5}$$

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

$$i\sum_{j=1}^{n}\omega_{kj}\dot{z}_j^* = -\frac{\partial H_{cl}}{\partial z_k}\ ,\ i\sum_{j=1}^{n}\omega_{jk}\dot{z}_j = \frac{\partial H_{cl}}{\partial z_k^*}\ , \tag{6}$$

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

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

where $\lambda_{jk} = -i(\Omega^*)^{-1}$ and $()^t$ refers to the transpose of the matrix. Thus, the variational principle for S applied on $\widehat{\mathcal{M}}$ leads to the following classical Liouville equations of motion [22]:

$$\frac{dz_j}{dt} = \{z, H_{cl}\}\ ,\ \frac{dz_j^*}{dt} = \{z^*, H_{cl}\}\ , \tag{7}$$

with H_{cl} defined by eq. (2), and $H_{cl}(z, z^*)$ is the expected value of the quantum Hamiltonian in the state represented by $\psi(z) \in \widehat{\mathcal{M}}$. Hence H_{cl} is considered the classical Hamiltonian associated to the quantum Hamiltonian H. Such association is usually called *dequantization* [30].

2.3. DYNAMICAL SYMMETRY GROUPS FOR 3D ION TRAPS

The group of canonical linear transformations for a dynamical system with n degrees of liberty is the symplectic group $Sp(2n, \mathbb{R})$. An electrically charged particle confined within an 3D ion trap can be explicitly described by the choerent states for a subgroup $\mathcal{G}$ of the symplectic group $Sp(6, \mathbb{R})$ [4]. Symplectic transformations in $\mathcal{S}p(2n, \mathbb{R})$ leave invariant the canonical form of the classical Hamiltonian equations of motion [31]. For a particle of mass M and electric charge Q trapped within a magnetic field, homogeneous along the axial direction x_3, and superimposed over an electric field obtained from the harmonic potential

$$V = \sum_{i,j=1}^{3}\zeta_{ij}x_i x_j\ , \tag{8}$$

with ζ_{ij} constant coefficients or time periodic functions which satisfy $\zeta_{11}+\zeta_{22}+\zeta_{33}=0$. The corresponding quantum Hamilton function can be expressed as

$$H=\frac{1}{2M}\sum_{j=1}^{3}p_j^2+QV+\frac{M}{8}\omega_c^2(x_1^2+x_2^2)-\frac{\omega_c}{2}(x_1p_2-x_2p_1)\ , \tag{9}$$

where $\omega_c=QB_0/M$ is the cyclotronic frequency for a Penning trap, B_0 is the homogeneous axial magnetic field, and the momentum operators are $p_j=-i\hbar\partial/\partial x$, $1\leq j\leq 3$. As the H_2 Hamiltonian is a polynomial of degree two in x_j and p_j, the corresponding dynamical group is a subgroup of the $Sp(6,\mathbb{R})$ group. Hence the coherent states that describe an electrically charged particle confined within a harmonic 3D ion trap can be expressed as $\Psi_u=\exp(iP_u)\,\Phi$, where P_u is a polynomial of degree two in x_j and p_j, with $1\leq j\leq 3$, the u index is a point in the classical phase, and Φ is a fixed state vector.

We enumerate the dynamical groups $\mathcal{G}$ associated to the most frequently use quadrupole trap geometries, with $\zeta_{ij}=0\,(i\neq j)$:

a) Paul trap with cylindrical symmetry $\zeta_{11}=\zeta_{22}$, $B_0=0\longmapsto\mathcal{G}=S_{rl}\otimes S_3\otimes SO(2)$

b) Elliptical Paul trap $\zeta_{11}\neq\zeta_{22}\neq\zeta_{33}$, $B_0=0\longmapsto\mathcal{G}=S_1\otimes S_2\otimes S_3$

c) Linear Paul trap $\zeta_{11}=-\zeta_{22}$, $B_0=0\longmapsto\mathcal{G}=S_1\otimes S_2$

d) Penning trap $\zeta_{11}=\zeta_{22}\longmapsto\mathcal{G}=S_{rl}\otimes S_3\otimes SO(2)$

e) Combined (Paul and Penning) trap $\zeta_{11}=\zeta_{22}\longmapsto\mathcal{G}=S_{rl}\otimes S_3\otimes SO(2)$

For $1\leq j\leq 3$ we have denoted by S_j the group linear canonical transformations in phase space (x_j,p_j), where $SO(2)$ is the rotations group aroud the x_3 axis, and S_{rl} is the group linear canonical transformations in phase space (x_1,p_1,x_2,p_2) reduced through $SO(2)$ (for fixed orbital angular momentum). The group linear canonical transformations consists of translations, rotations and squeezes in phase space. Thus, a deeper understanding of the uncertainty principle is possible by means of canonical transformations within the phase space picture of quantum mechanics.

2.4. ION DYNAMICS WITHIN A 3D QUADRUPOLE PENNING TRAP

The equations of motion for an ion of mass M and electric charge Q, confined within an 3D quadrupole Penning trap, are

$$M\ddot{\vec{\boldsymbol{r}}}=Q\vec{\boldsymbol{E}}+Q\dot{\vec{\boldsymbol{r}}}\times\vec{\boldsymbol{B}}\ , \tag{10}$$

where $\vec{\boldsymbol{E}}=-\bigtriangledown\Phi$ represents the electric field, and $\vec{\boldsymbol{B}}$ stands for the magnetic field. The electric potential is chosen as

$$\Phi\left(\vec{\boldsymbol{r}},t\right)=A\left(t\right)f\left(\vec{\boldsymbol{r}}\right)\ , \tag{11}$$

where A is a constant or a continuous function of period $T = 2\pi/\Omega$, while f satisfies the Laplace equation $\Delta f = 0$. The classical Hamilton function for an ion confined within a quadrupole trap is

$$H = \frac{1}{2M}\left[\vec{\boldsymbol{p}} - Q\vec{\boldsymbol{A}}\right]^2 + Q\Phi \ . \tag{12}$$

We have denoted by $\vec{\boldsymbol{A}}$ the vector potential of the magnetic field, and by $\vec{\boldsymbol{r}} = (x, y, z)$ the position vector of the ion. The momentum $\vec{\boldsymbol{p}} = (p_x, p_y, p_z)$ and angular momentum vectors $\vec{L}$ are

$$\vec{\boldsymbol{p}} = M\dot{\vec{\boldsymbol{r}}} + Q\vec{\boldsymbol{A}} \ , \ \vec{\boldsymbol{L}} = M\vec{\boldsymbol{r}} \times \dot{\vec{\boldsymbol{r}}} + Q\vec{\boldsymbol{r}} \times \vec{\boldsymbol{A}} \ . \tag{13}$$

The corresponding Hamilton equations of motion are

$$\dot{\vec{\boldsymbol{r}}} = \nabla_{\vec{\boldsymbol{p}}} H \ , \ \dot{\vec{\boldsymbol{p}}} = -\nabla_{\vec{\boldsymbol{r}}} H \ . \tag{14}$$

Further on we will consider a uniform axial magnetic field $\vec{\boldsymbol{B}} = (0, 0, B_0)$, such as the case of a Penning trap. By choosing $\vec{\boldsymbol{A}} = \frac{1}{2}\vec{\boldsymbol{B}} \times \vec{\boldsymbol{r}}$, and using $\vec{\boldsymbol{B}} = \bigtriangledown \times \vec{\boldsymbol{A}}$, the Hamiltonian described by eq. (12) becomes

$$H = \frac{1}{2M}\left[\vec{p}^2 + QB_0\left(yp_x - xp_y\right) + \frac{1}{4}Q^2B_0^2\left(x^2 + y^2\right)\right] + Q\Phi\left(\vec{\boldsymbol{r}}, t\right) \ . \tag{15}$$

The Hamilton equations of motion (14) for a trapped ion can be expressed as

$$M\ddot{x} = QB_0\dot{y} - Q\frac{\partial\Phi}{\partial x} \ , \ M\ddot{y} = -QB_0\dot{x} - Q\frac{\partial\Phi}{\partial y} \ , \ M\ddot{z} = -Q\frac{\partial\Phi}{\partial z} \ . \tag{16}$$

As the Hamiltonian described by eq. (15) exhibits axial symmetry, it is convenient to introduce the cylindrical coordinates ρ, θ and z, with $x = \rho\cos\theta$ and $y = \rho\sin\theta$. Hence we can rewrite the first two equations in (16) as

$$\ddot{\rho} = \frac{1}{\rho^3}\left(\frac{L_z}{M}\right)^2 - \frac{\omega_c^2}{4}\rho - \frac{Q}{M}\frac{\partial\Phi}{\partial\rho} \ , \tag{17}$$

$$\rho^2\ddot{\theta} = -2\rho\dot{\rho}\dot{\theta} - \omega_c\rho\dot{\rho} - \frac{Q}{M}\frac{\partial\Phi}{\partial\theta} \ , \tag{18}$$

with $\rho = \sqrt{x^2 + y^2}$, and $\omega_c = QB_0/M$ is the cyclotronic frequency for an ion confined within a Penning trap. In case of a cylindrical symmetry trap the electric potential Φ does not depend on θ. Therefore the projection of the angular moment L_z along the z axis is a constant of the motion in case of axial (cylindrical) symmetry

$$L_z = M\rho^2\dot{\theta} + \frac{Q}{2}\rho^2B_0 \ . \tag{19}$$

If we use complex coordinates $z = x + iy$ and $z^* = x - iy$, we obtain the following equations of motion

$$\ddot{z} = -i\omega_c \dot{z} - 2\frac{Q}{M}\frac{\partial \Phi}{\partial z^*} \tag{20a}$$

$$\ddot{z}^* = i\omega_c \dot{z}^* - 2\frac{Q}{M}\frac{\partial \Phi}{\partial z} \tag{20b}$$

3. COHERENT STATES FOR AN ION CONFINED WITHIN A QUADRUPOLE TRAP WITH CYLINDRICAL SYMMETRY

3.1. LIE ALGEBRAS ASSOCIATED TO THE $Sp(2,\mathbb{R})$ SYMPLECTIC GROUP

We investigate the quantum Hamilton function for a charged particle of mass M and electric charge Q, confined within a quadrupole 3D ion trap that exhibits cylindrical symmetry

$$H_2 = \frac{1}{2M}\left(-i\hbar\boldsymbol{\nabla} - \frac{Q}{2}\boldsymbol{B}\times\boldsymbol{r}\right)^2 + QA(t)\left(x^2 + y^2 - 2z^2\right) . \tag{21}$$

we have denoted by $\boldsymbol{r} = (x, y, z)$ the position operator. As shown in 2.4, in case of a Penning trap A is a constant. For an electrodynamic (Paul) trap, $A(t)$ is a time periodic function, of period $2\pi/\Omega$, where Ω represents the a.c. trapping voltage frequency (radiofrequency-RF). In particular, the Paul trap is characterized by the absence of the magnetic field $B_0 = 0$, and

$$A(t) = (r_0^2 + 2z_0^2)^{-1}\left(U_0 + V_0\cos\Omega t\right), \tag{22}$$

where r_0 and z_0 represent the radial and axial semiaxes of the 3D ion trap electrodes.

As the H_2 Hamiltonian commutes with the axial angular moment [10]

$$L_z = i\hbar\left(y\frac{\partial}{\partial x} - x\frac{\partial}{\partial y}\right) , \tag{23}$$

our investigation will be limited to the eigenvector space of the L_z operator, with fixed eigenvalue $\hbar l$, where l is a positive integer and it stands for the quantum orbital number. The Hamiltonian reduced to this subspace can be expressed as [10, 12]

$$H_{2l} = H_a + H_r - \frac{\hbar\omega_c}{2}l , \tag{24}$$

where H_a and H_r are the axial, respectively the radial motion Hamiltonians, defined as:

$$H_a = -\frac{\hbar^2}{2M}\frac{\partial^2}{\partial\rho^2} + \frac{M}{2}\mu_a z^2 , \tag{25}$$

$$H_r = -\frac{\hbar^2}{2M}\left(\frac{\partial^2}{\partial\rho^2} + \frac{1}{\rho}\frac{\partial}{\partial\rho} - \frac{l^2}{\rho^2}\right) + \frac{M}{2}\mu_r\rho^2, \tag{26}$$

with $\rho = \sqrt{x^2+y^2}$ and

$$\mu_a = -\frac{4Q}{M}A\ , \quad \mu_r = \frac{1}{4}\left(\omega_c^2 - 2\mu_a\right)\ , \quad \omega_c = \frac{Q}{M}B_0\ . \tag{27}$$

We now introduce the Lie algebra generators for the axial and radial symplectic groups [10, 12, 27]

$$K_{0a} = \frac{1}{4}\left(-\frac{\partial^2}{\partial z^2} + z^2\right)\ , \quad K_{1a} = \frac{1}{4}\left(\frac{\partial^2}{\partial z^2} + z^2\right)\ , \tag{28}$$

$$K_{0r} = \frac{1}{4}\left[-\frac{\partial^2}{\partial \rho^2} + \rho^2 + \left(l^2 - \frac{1}{4}\right)\frac{1}{\rho^2}\right]\ , \tag{29a}$$

$$K_{1r} = \frac{1}{4}\left[\frac{\partial^2}{\partial \rho^2} + \rho^2 - \left(l^2 - \frac{1}{4}\right)\frac{1}{\rho^2}\right]\ . \tag{29b}$$

The K_{0j}, K_{1j} and $K_{2j} = i[K_{1j}, K_{0j}]$ satisfy the commutation relations with respect to the Lie algebra of the $Sp(2,\mathbb{R})$ group:

$$[K_{0j}, K_{1j}] = iK_{2j}\ , \quad [K_{2j}, K_{0j}] = iK_{1j}\ , \quad [K_{2j}, K_{1j}] = iK_{0j}\ ,\ j = a, r\ . \tag{30}$$

These operators span the Lie algebra associated to the Lie group $\mathcal{G}_j$, which results as an unitary irreducible representation (UIR) of the symplectic group $Sp(2,\mathbb{R})$ of Bargmann index $k_a = \frac{1}{4}, \frac{3}{4}$ and $k_r = (l+1)/2$ [34, 35].

Both the axial H_a and radial H_r Hamiltonians are linear combinations of the Lie algebra generators [4, 7, 9, 10]:

$$H_j = \alpha_j K_{0j} + \beta_j K_{1j}\ , \quad j = a, r\ , \tag{31}$$

where

$$\alpha_j = M\mu_j + \frac{\hbar^2}{M}\ , \quad \beta_j = M\mu_j - \frac{\hbar^2}{M}\ . \tag{32}$$

Hence, we obtain that $\mathcal{G}_a$ is the dynamical group for the axial Hamiltonian H_a, and $\mathcal{G}_r$ is the dynamical group associated to the radial Hamiltonian H_r. Moreover, $\mathcal{G} = \mathcal{G}_a \otimes \mathcal{G}_r \otimes SO(2)$ is the dynamical group associated to the quantum Hamiltonian H_2. We have denoted by $SO(2)$ the rotations group generated by the axial angular moment operator L_z.

3.2. ION CONFINED IN A NONLINEAR, AXIALLY SYMMETRIC 3D TRAP

We choose an electric potential for the trap that exhibits axial symmetry [4, 32]

$$\Phi\left(\vec{r}, t\right) = A(t) g\left(\rho, z\right)\ , \tag{33}$$

where $A(t)$ is a time periodic function, of period $T = 2\pi/\Omega$, and g is a function of ρ^2 and z^2

$$g(\rho, z) = \sum_{k\geq 1} c_k H_{2k}(\rho, z) \ , \tag{34}$$

where c_k are constants, and the H_{2k} polynomials are the spherical harmonic functions of degree k in ρ^2 and z^2, defined as

$$H_{2k}(\rho, z) = \sum_{n=0}^{k} \frac{(2k)!\rho^{2n} z^{2(k-n)}}{4^n (2k-2n)! (n!)^2} \ . \tag{35}$$

The electric potential described by eq. (33) is characteristic to a 3D ion trap that exhibits both axial symmetry (in ρ and z), and symmetry with respect to the radial xOy plan. In case of a Penning trap A is constant in time, but for most RF (Paul) traps $A(t) = U_0 + V_0 \cos\Omega t$, where U_0 is the d.c. voltage and V_0 is the a.c. (RF) trapping voltage. In case of harmonic potentials $c_k = 0$,for $k > 1$

$$g(\rho, z) = \frac{1}{r_0^2 + 2z_0^2} \left(\rho^2 - 2z^2\right) \ , \ c_2 = -\frac{1}{r_0^2 + 2z_0^2} \ , \tag{36}$$

where r_0 and z_0 represent the semiaxes of the quadrupole trap, and $\rho^2 = x^2 + y^2$. The particular case of an ideal Paul trap is obtained for zero magnetic field. In case of a nonlinear octupole trap, the electric potential given by eq. (34) becomes [32]

$$g(\rho, z) = \frac{c_1}{4} H_2(\rho, z) + \frac{c_2}{8} H_4(\rho, z) + \dots \ ,$$
$$H_2(\rho, z) = 2z^2 - \rho^2 \ , \ H_4(\rho, z) = 8z^4 - 24z^2\rho^2 + 3\rho^4 \ . \tag{37}$$

The quantum Hamiltonian for a charged particle characterized by an angular moment $\hbar l$, confined within an axially symmetric electrodynamic trap can be expressed as

$$H_l = H_{2l} + QA(t) P\left(\rho^2, z^2\right), \tag{38}$$

where H_{2l} is given by eq. (24), and the nonharmonic part is defined by the polynomial

$$P\left(\rho^2, z^2\right) = \sum_{k\geq 2} c_k H_{2k}(\rho, z) \ . \tag{39}$$

Using equations (28), (3.1) and (31) we infer

$$\rho^2 = 2(K_{0r} + K_{1r}), \quad z^2 = 2(K_{0a} + K_{1a}) \ . \tag{40}$$

We investigate the Schrödinger equation

$$i\hbar \frac{\partial \chi}{\partial t} = H_l \chi \ , \tag{41}$$

where the quantum Hamilton function H_l results from eq. (38), which we particularize for combined quadrupole and octupole traps. Thus, the quantum Hamilton

function describes an algebraic model if $P\left(\rho^2, z^2\right)$ is a polynomial function. Such model is linear for quadrupole traps (P is a linear combination of ρ^2 and z^2), where we have a pure quadrupole field which is the ideal situation. Real traps do not exhibit a pure quadrupole field, which is why mitigation techniques are implemented, and the effect of the nonlinear termis in the series expansion of the electric potential has to be considered.

We also introduce the elastic constants

$$K_r = \frac{M\omega_c^2}{4} - 2Qc_2A(t)\ ,\ K_a = 4Qc_2A(t) \tag{42}$$

As shown in [27], the quantum Hamilton function that describes a trapped electrically charged ion (particle) of electric charge Q, mass M, and orbital angular momentum $\hbar l$ in case of a 3D quadrupole trap with octupole anharmonicity, can be expressed as

$$\begin{aligned} H_l = \hbar\omega_r\left(K_{0r} - K_{1r}\right) + 2\hbar\omega_a\left(K_{0a} - K_{1a}\right) + \frac{K_r}{2}\frac{2\hbar}{M\omega_r}\left(K_{0r} + K_{1r}\right) \\ + \frac{K_a}{2}\frac{2\hbar}{M\omega_a}\left(K_{0a} + K_{1a}\right) - \frac{\omega_c}{2}\hbar l + QA\left(t\right)P\left(\rho^2, z^2\right)\ . \end{aligned} \tag{43}$$

Hence the study of the Hamilton function for an ion trapped within the combined 3D trap we have considered is reduced to the study of the linear Hamilton system for the real symplectic group $Sp\left(2, \mathbb{R}\right)$. Then

$$P\left(\rho^2, z^2\right) = D_4H_4\left(\rho, z\right) = D_4\left(8z^4 - 24z^2\rho^2 + 3\rho^4\right)$$

where D_4 stands for a coefficient that depends on the trap geometry. We perform an average on the generators of the symplectic group and on ρ^4, ρ^2z^2 and z^4. The anharmonic term is

$$\Phi_{anh} = A\left(t\right)D_4H_4\left(\rho, z\right)\ ,$$

while in the quasipotential approximation case (ideal Paul trap), the anharmonic term can be expressed as

$$\Phi_{anheff} = C_4H_4\left(\rho, z\right) + C_6H_6\left(\rho, z\right)\ ,$$

where the C_4 and C_6 coefficients depend on the specific trap geometry. Therefore, the quantum Hamilton function is

$$H_l = H_{anh} + \left\{ \begin{array}{ll} Q\Phi_{anh} & \text{Paul and Penning trap} \\ Q\Phi_{anheff} & \text{ideal Paul trap} \end{array} \right\} \tag{44}$$

Eq. (44) gives the quantum Hamilton function for the particular traps we have chosen, including the pseudopotential approximation case that characterizes an ideal Paul trap.

3.3. SCHRÖDINGER EQUATION SOLUTIONS AND ENERGY SPECTRUM

The solution of the Schrödinger equation for the H_2 Hamiltonian can be expressed as [4, 12]

$$\Psi(\rho,z,\theta)=\frac{1}{\sqrt{\rho}}\exp\left[il\left(\theta+\frac{\omega_c}{2}t\right)\right]\Psi_r(\rho)\,\Psi_a(z)\,, \tag{45}$$

where

$$i\hbar\frac{\partial\Psi_j}{\partial t}=H_j\Psi_j\,,\quad j=a,r\,. \tag{46}$$

The solutions of the Schrödinger equation for the H_l Hamiltonian given by eq. (43) can be expressed as [4, 12]

$$\Psi_{k_am_ak_rm_rl}=\frac{1}{\sqrt{\rho}}\exp\left[il\left(\theta+\frac{\omega_c}{2}t\right)-i\varphi\right]\psi_{k_am_a}(z_a)\psi_{k_rm_r}(z_r)\,, \tag{47}$$

unde $m_a,m_r\in\mathbb{N}$ are natural numbers, z_a and z_r represent complex coordinates within the unit disk [8] ($|z_a|<1$, $|z_r|<1$), and $\varphi\in\mathbb{R}$ is a phase obtained from the equation

$$\varphi=(k_a+m_a)\,\varphi_a+(k_r+m_r)\,\varphi_r\,. \tag{48}$$

The variables z_a,z_r,φ_a, and φ_r are solutions of the differential equations

$$i\frac{dz_j}{dt}=\alpha_j+\frac{\beta_j}{2}\left(z_j^2+1\right)\,,\ \frac{d\varphi_j}{dt}=\alpha_j+\frac{\beta_j}{2}\left(z_j+z_j^*\right)\quad j=a,r\,. \tag{49}$$

The eigenfunctions $\psi_{k_am_a}(z_a)$ and $\psi_{k_rm_r}(z_r)$ represent symplectic coherent vectors for the Lie groups $\mathcal{G}_a$ and $\mathcal{G}_r$. In order to define them we introduce the ladder operators $K_{\pm j}=K_{1j}\pm iK_{2j}$, and the canonical base

$$\phi_{k_jm_j}=\left[\frac{\Gamma(2k_j)}{m_j!\Gamma(2k_j+m_j)}\right]^{1/2}(K_{+j})^{m_j}\,\phi_{k_j0}\,, \tag{50}$$

where the normalized vector satisfies $K_{+j}\phi_{k_j0}=k_j\phi_{k_j0}$, and $K_{-j}\phi_{k_j0}=0$.

We also introduce the unitary evolution operators

$$U(z_j)=\exp(z_jK_{+j})\exp(\lambda_jK_{0j})\exp\left(-z_j^*K_{-j}\right)\,, \tag{51}$$

where $\lambda_j=\ln(1-z_jz_j^*)$. The coherent symplectic vectors are defined as

$$\psi_{k_jm_j}(z_j)=U(z_j)\,\phi_{k_jm_j}\,,\quad j=a,r\,. \tag{52}$$

The quasienergy spectrum is determined by the functions $\Psi_{k_am_ak_rm_rl}$ and the quasienergies

$$E_{k_am_ak_rm_rl}=2\hbar\left[\chi_a(k_a+m_a)+\chi_r(k_r+m_r)-\frac{\omega_j}{4}l\right]\,, \tag{53}$$

where χ_a and χ_r are the Floquet exponents for the stable solutions of the Hill equations

$$\frac{d^2u_j}{dt^2} + \mu_j w_j = 0 \,. \tag{54}$$

4. QUASICLASSICAL DYNAMICS IN NONLINEAR 3D COMBINED AND PAUL TRAPS

4.1. CLASSICAL HAMILTON FUNCTION FOR AN ANHARMONIC TRAP. EQUATION OF MOTION

We denote $\Omega_\varepsilon = K_0 + \varepsilon K_1 = K_0 + \frac{\varepsilon}{2}(K_+ + K_-)$, with $\varepsilon = \pm 1$. Using eq. (52) and the Baker-Campbell-Hausdorff relation [9, 26, 35], we infer

$$U^\dagger(z)\,\Omega_\varepsilon U(z) = \frac{(1+\varepsilon z)(1+\varepsilon z^*)}{(1-zz^*)} E_\varepsilon \,, \tag{55}$$

where $U^\dagger$ represents the Hermitian adjoint of the unitary operator $U(z)$, and

$$E_\varepsilon = \frac{1}{2}(1-zz^*)^{-1}\left[2(1+z)(1+z^*)K_0 + \varepsilon(1+z^*)^2 K_- + \varepsilon(1+z)^2 K_+\right] . \tag{56}$$

Moreover, using eqs. (55) and (56) we obtain

$$\langle z,k,m|\Omega_\varepsilon^n|z,k,m\rangle = \left[\frac{(1+\varepsilon z)(1+\varepsilon z^*)}{1-zz^*}\right]^n \langle k,m|E_\varepsilon^n|k,m\rangle \,. \tag{57}$$

The expressions for E^2 and E^3 are obtained are quite complex and, for the sake of simplicity, we will not provide them here. We weight on the vacuum state vector $|0\rangle$

$$K_-|0\rangle = 0 \,,\ \langle 0|0\rangle = 0 \,,\ K_0|0\rangle = k|0\rangle \,,\ \langle 0|K_+ = 0 \,. \tag{58}$$

Then, the Casimir operator can be expressed as

$$C_2 = K_0^2 - \frac{1}{4}(K_+ + K_-)^2 - \frac{1}{4i^2}(K_+ - K_-)^2 = k(k-1) \,,$$

and

$$K_+K_- + K_-K_+ = 2K_0^2 - 2k(k-1) \tag{59}$$

Using eqs. (58) we infer

$$\left\langle E^2\right\rangle = \left\langle 0|E^2|0\right\rangle = 4k^2 + 2k \,, \tag{60a}$$

$$\left\langle E^3\right\rangle = \left\langle 0|E^3|0\right\rangle = 8k^3 + 12k^2 + 4k \,. \tag{60b}$$

If instead of the vacuum state vector $|0\rangle$ we weight on a vector of an orthonormal system of state vectors $|k,m\rangle$, namely $\langle k,m|k,m'\rangle = \delta_{mm'}$, we obtain

$$\left\langle k,m|E^2|k,m\right\rangle = 2k(2k+1) + 12km + 6m^2 \,, \tag{61a}$$

$$\left\langle k,m|E^3|k,m\right\rangle = 4k\left(k+1\right)\left(2k+1\right)+4mk\left(5+12k\right)+4m^2\left(15k+1\right)+20m^3\ , \tag{61b}$$

where $K_0\left|k,m\right\rangle = \left(k+m\right)\left|k,m\right\rangle$ [10] and we make use of eqs. (58) and (60). From eq. (57) [4, 10] we infer

$$\left\langle z,k,m|K_0-K_1|z,k,m\right\rangle = \left(k+m\right)\frac{\left(1-z\right)\left(1-z^*\right)}{1-zz^*}\ , \tag{62}$$

where z stands for the squeezed state parameter, k and m represent pure harmonic oscillator states, while K_0-K_1 is the kinetic energy. The classical energy (Hamilton) function described by eq. (43), can be now expressed as

$$\begin{aligned}\mathcal{H}_{cl} = \hbar\omega_r\left(k_r+m_r\right)\frac{\left(1-z_r\right)\left(1-z_r^*\right)}{1-z_rz_r^*}+2\hbar\omega_a\left(k_a+m_a\right)\frac{\left(1-z_a\right)\left(1-z_a^*\right)}{1-z_az_a^*}+\\ \frac{2\hbar K_r}{M\omega_r}\left(k_r+m_r\right)\frac{\left(1-z_r\right)\left(1-z_r^*\right)}{1-z_rz_r^*}+\frac{2\hbar K_a}{M\omega_a}\left(k_a+m_a\right)\frac{\left(1-z_a\right)\left(1-z_a^*\right)}{1-z_az_a^*}+\\ H_{anh}-\frac{\omega_c}{2}\hbar l\ ,\end{aligned} \tag{63}$$

where

$$H_{anh} = QA\left(t\right)\left\langle P\left(\rho^2,z^2\right)\right\rangle = QA\left(t\right)\sum_{k\geq 1}c_k\langle H_{2k}\rangle. \tag{64}$$

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

$$H_{anh} = \begin{cases} QA\left(t\right)D_4\left\langle H_4\right\rangle, & \text{Paul and Penning trap case,}\\ QC_4\left\langle H_4\right\rangle + QC_6\left\langle H_6\right\rangle, & \text{pseudopotential approx. case - RF trap.}\end{cases} \tag{65}$$

The second term in eq. (65) characterizes the pseudopotential case (the radiofrequency or Paul trap). Then

$$\left\langle H_4\right\rangle = 8S_{2a}-24S_{1r}S_{1a}+3S_{2r}\ , \tag{66}$$

$$\left\langle H_6\right\rangle = 16S_{3a}-120S_{2a}S_{1r}+90S_{1a}S_{2r}-5S_{3r}\ , \tag{67}$$

The parameter values are known $k_a=\frac{1}{4},\frac{3}{4}\ ;\ m_a,m_r=0,1,\ldots\ ;\ k_r=\frac{l+1}{2}$, where the orbital angular momentum is $L^2=l\left(l+1\right)I$. By minimizing $\mathcal{H}_{cl}$ after z, we infer the approximations for the quantum energies. Using cylindrical coordinates $\left(z=\rho e^{i\theta}\ ,\ z^*=\rho e^{-i\theta}\right)$, we introduce the complex variables

$$\xi_j = \frac{\left(1+z\right)\left(1+z^*\right)}{1-zz^*}\quad ,\quad \eta_j = \frac{\left(1-z\right)\left(1-z^*\right)}{1-zz^*}\ ,\ j=a,r\ . \tag{68}$$

We denote

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

where

$$S_j(z,k,m) = \left[\frac{(1+z)(1+z^*)}{1-zz^*}\right]^j Q_j(k,m) = \xi^j Q_j(k,m) \ . \tag{69}$$

Moreover

$$S_1(z,k,m) = 2\xi(k+m) \tag{70a}$$

$$S_2 = \xi^2\left[2k(2k+1)+12km+6m^2\right] \tag{70b}$$

$$S_3 = \xi^3\left[4k(k+1)(2k+1)+4mk(5+12k)+4m^2(15k+1)+20m^3\right] \ . \tag{70c}$$

$$Q_1(k,m) = 2(k+m) \tag{71a}$$

$$Q_2(k,m) = 2k(2k+1)+12km+6m^2 \tag{71b}$$

$$Q_3(k,m) = 4k(k+1)(2k+1)+4mk(5+12k)+4m^2(15k+1)+20m^3 \ . \tag{71c}$$

Hence, the classical Hamiltonian (Husimi function) for an anharmonic (octupole) trap can be expressed as

$$\begin{aligned}\mathcal{H}_{cl} = {} & A_r\eta_r + A_a\eta_a + B_r\xi_r + B_a\xi_a + \left(C\xi_r^2 + C'\xi_r\xi_a + C"\xi_a^2\right) \\ & + \left(D_{30}\xi_r^3 + D_{21}\xi_r^2\xi_a + D_{12}\xi_r\xi_a^2 + D_{03}\xi_a^3\right) - \frac{\omega_c}{2}\hbar l \ .\end{aligned} \tag{72}$$

If the anharmonic part P is a polynomial in ρ^2 and z^2, then the classical Hamiltonian H_{cl} given by eq. (72) is a polynomial in ξ_a and ξ_r. In order to find the minimum points of the Hamilton (Husimi) function, we solve

$$\frac{\partial\mathcal{H}}{\partial\xi_a} = 0 \ , \ \frac{\partial\mathcal{H}}{\partial\xi_r} = 0 \ , \ \frac{\partial\mathcal{H}}{\partial\eta_a} = 0 \ , \ \frac{\partial\mathcal{H}}{\partial\eta_r} = 0 \ .$$

Then, the classical Hamilton function for an anharmonic octupole trap can be expressed as

$$\begin{aligned}\mathcal{H}_{cl} = {} & \hbar\omega_r(k_r+m_r)\eta_r + 2\hbar\omega_a(k_a+m_a)\eta_a + \\ & \frac{2\hbar K_r}{M\omega_r}(k_r+m_r)\xi_r + \frac{2\hbar K_a}{M\omega_a}(k_a+m_a)\xi_a - \frac{\omega_c}{2}\hbar l +\end{aligned} \tag{73}$$

$$\begin{cases} QA(t)\,D\,[8S_{2a}-24S_{1r}S_{1a}+3S_{2r}] \\ QC_4\,(8S_{2a}-24S_{1r}S_{1a}+3S_{2r})+QC_6\,(16S_{3a}-120S_{2a}S_{1r}+90S_{1a}S_{2r}-5S_{3r})\,, \end{cases}$$

where the first term refers to the case of a combined trap, while the second case describes the pseudopotential approximation in case of an ideal Paul trap. Such pseudopotential is the outcome of micromotion kinetic energy. The energy function associated to the quantum Hamilton function H_l is a classical type Hamiltonian H_{cl}, whose values represent exactly the expected values of H_l on the coherent states $\psi_{k_a 0}(z_a)$ and $\psi_{k_r 0}(z_r)$. Hence, we can ascertain that quantum dynamics of trapped ions can be characterized by solutions of the Schrödinger equation, where the $H = H_r$ Hamilton function corresponds to radial motion, while $H = H_a$ is associated to the axial motion. We notice that the classical Hamilton function results from the TDVP applied on coherent states

$$\mathcal{H}_{cl} = \langle z, k, m | H_l | z, k, m \rangle \ ,$$

and it determines an equation of motion in the classical Lobacevski phase space $|z_j| < 1$:

$$\dot{z}_j = \{z_j, \mathcal{H}_{cl}\} \ , \ j = a, r \ . \tag{74}$$

where $\{,\}$ stands for the generalized Poisson bracket. We finally obtain

$$\{z_j, \mathcal{H}_{cl}\} = \frac{\left(1 - z_j z_j^*\right)^2}{2i\,(k+m)} \frac{\partial \mathcal{H}_{cl}}{\partial z_j^*} \ , \tag{75}$$

which represents the equation of motion for an ion confined within a combined (Paul) trap.

4.1.1. Classical Hamilton function for an anharmonic combined trap

According to eq. (73) the Hamilton function expression is

$$\mathcal{H}_{cl\ anh} = \hbar\omega_r\,(k_r+m_r)\,\eta_r + 2\hbar\omega_a\,(k_a+m_a)\,\eta_a + \frac{2\hbar K_r}{M\omega_r}\,(k_r+m_r)\,\xi_r + \frac{2\hbar K_a}{M\omega_a}\,(k_a+m_a)\,\xi_a - \frac{\omega_c}{2}\hbar l + QA(t)\,D\,[8S_{2a}-24S_{1r}S_{1a}+3S_{2r}] \ . \tag{76}$$

The expressions for S_{1a}, S_{2a}, S_{1r} and S_{2r} are given by eqs. (70a). We turn to the expression of the Hamilton function described by eq. (76). The points of minimum of the Hamilton function are described by the following equations

$$\frac{2\hbar K_a}{M\omega_a}\,(k_a+m_a) + QA(t)\,D_4\,[16\xi_a \cdot Q_2\,(k_a,m_a) - 96\xi_r\,(k_a+m_a)\,(k_r+m_r)] = 0 \tag{77a}$$

$$\frac{2\hbar K_r}{M\omega_r}\left(k_r+m_r\right)+QA\left(t\right)D_4\left[-96\xi_a\left(k_a+m_a\right)\left(k_r+m_r\right)+6\xi_rQ_2\left(k_r,m_r\right)\right]=0 \tag{77b}$$

$$2\hbar\omega_{a,r}\left(k_{a,r}+m_{a,r}\right)=0 \tag{77c}$$

4.1.2. Quasipotential approximation case - Ideal RF (Paul) trap case

According to eq. (73), the expression of the classical Hamilton function for an octupole trap, in case of the pseudopotential approximation is

$$\mathcal{H}_{cl\ anheff}=\hbar\omega_r\left(k_r+m_r\right)\eta_r+2\hbar\omega_a\left(k_a+m_a\right)\eta_a+\frac{2\hbar K_r}{M\omega_r}\left(k_r+m_r\right)\xi_r + \frac{2\hbar K_a}{M\omega_a}\left(k_a+m_a\right)\xi_a-\frac{\omega_c}{2}\hbar l+QC_4<H_4>+QC_6<H_6> \tag{78}$$

where H_4 and H_6 are characterized by eqs. (66 - 67). Hence

$$S_{3a}=4k_a\left(k_a+1\right)\left(2k_a+1\right)+4k_am_a\left(5+12k_a\right)+4m_a^2\left(15k_a+1\right)+20m_a^3 \tag{79}$$

$$S_{3r}=4k_r\left(k_r+1\right)\left(2k_r+1\right)+4k_rm_r\left(5+12k_r\right)+4m_r^2\left(15k_a+1\right)+20m_r^3 \tag{80}$$

The points of minimum that characterize equilibrium configurations are given by the equations

$$\frac{2\hbar K_a}{M\omega_a}\left(k_a+m_a\right)+QC_4\left[16\xi_aQ_2\left(k_a,m_a\right)-96\xi_r\left(k_a+m_a\right)\left(k_r+m_r\right)\right]+ QC_6[48\xi_a^2Q_3\left(k_a,m_a\right)-240\xi_a\xi_rQ_2\left(k_a,m_a\right)Q_1\left(k_r,m_r\right)+ 90\xi_rQ_1\left(k_a,m_a\right)Q_2\left(k_r,m_r\right)]=0 \tag{81}$$

$$\frac{2\hbar K_r}{M\omega_r}\left(k_r+m_r\right)+QC_4\left[-96\xi_a\left(k_a+m_a\right)\left(k_r+m_r\right)+6\xi_rQ_2\left(k_r,m_r\right)\right]+ QC_6[-120\,\xi_a^2Q_2\left(k_a,m_a\right)Q_1\left(k_r,m_r\right)+180\,\xi_a\xi_rQ_1\left(k_a,m_a\right)Q_2\left(k_r,m_r\right)- 15\xi_r^2Q_3\left(k_r,m_r\right)]=0\,. \tag{82}$$

In the pseudopotential approximation case, the points of minimum of the dequantified Hamilton function define the equilibrium configurations for trapped ions, of interest for implementing and scaling quantum logic [18, 20]. The possibility to use numerical simulations to investigate the associated (semi)classical or quantum dynamics for any kind of engineered quantum system represents an important issue, and the methods presented in [36] can be directly adapted to any given Hamiltonian that

describes a system of trapped ions. Simulations on time-dependent dynamics in RF ion traps can be generalized to multispecies ion crystals in general multipole traps, which leads to time-dependent quantum wavefunctions [37].

4.1.3. Classical equations of motion within an octupole 3D ion trap

We start from eqs. (68) then performing the math. We infer

$$\frac{\partial \mathcal{H}}{\partial z^*} = \frac{\partial \mathcal{H}}{\partial \xi}\left(\frac{1+z}{1-zz^*}\right)^2 - \frac{\partial \mathcal{H}}{\partial \eta}\left(\frac{z-1}{1-zz^*}\right)^2 \tag{83a}$$

$$\frac{\partial \mathcal{H}}{\partial z} = \frac{\partial \mathcal{H}}{\partial \xi}\left(\frac{1+z^*}{1-zz^*}\right)^2 - \frac{\partial \mathcal{H}}{\partial \eta}\left(\frac{z^*-1}{1-zz^*}\right)^2 . \tag{83b}$$

Further on we infer

$$2i\left(k+m\right)\dot{\xi} = 4\frac{z-z^*}{1-zz^*}\frac{\partial \mathcal{H}}{\partial \eta} . \tag{84a}$$

$$2i\left(k+m\right)\dot{\eta} = -4\frac{z-z^*}{1-zz^*}\frac{\partial \mathcal{H}}{\partial \xi} . \tag{84b}$$

We now return to eq. (68) and perform the math

$$\left(z-z^*\right)^2 = 16\frac{1-\xi\eta}{\left(\xi+\eta+2\right)^2} . \tag{85}$$

Hence

$$\frac{z-z^*}{1-zz^*} = i\varepsilon\sqrt{\left|1-\xi\eta\right|}\ ,\ \varepsilon = \pm 1 . \tag{86}$$

Considering eq. (86), the equations of motion (84a) and (84b) can be expressed as

$$2\left(k+m\right)\dot{\eta} = -4\varepsilon\sqrt{\left|1-\xi\eta\right|}\frac{\partial \mathcal{H}}{\partial \xi} \tag{87a}$$

$$2\left(k+m\right)\dot{\xi} = 4\varepsilon\sqrt{\left|1-\xi\eta\right|}\frac{\partial \mathcal{H}}{\partial \eta} . \tag{87b}$$

Further on, we denote

$$i\sigma = \frac{z-z^*}{1-zz^*} \Rightarrow -\sigma^2 = 1-\xi\eta\,, \tag{88}$$

while the time derivative is

$$2\sigma\dot{\sigma} = \dot{\xi}\eta + \xi\dot{\eta} . \tag{89}$$

Then eqs. (87a) and (87b) can be expressed as

$$\left(k+m\right)\dot{\eta} = -2\sigma\frac{\partial \mathcal{H}}{\partial \xi}\ ,\ \left(k+m\right)\dot{\xi} = 2\sigma\frac{\partial \mathcal{H}}{\partial \eta} . \tag{90}$$

By comparing eqs. (90) and (89), we infer

$$\left(k+m\right)\dot{\sigma} = \eta\frac{\partial \mathcal{H}}{\partial \eta} - \xi\frac{\partial \mathcal{H}}{\partial \xi} . \tag{91}$$

5. CONCLUSIONS

The TDVP method was applied on coherent state orbits, which yields to Hamilton type equations of motion on Kähler sub-manifolds such as classical phase spaces. Such formalism is developed and applied in the paper to characterize Hamilton functions that are nonlinear in the infinitesimal generators of a dynamical symmetry group (nonlinear 3D ion traps). The classical Hamilton equations of motion for a Penning trap are obtained, using both cylindrical and complex coordinates. The explicit expression of the quantum Hamilton function associated to an ion confined within an anharmonic 3D trap with cylindrical symmetry is obtained, as a function of the Lie algebra generators for the axial and radial symplectic groups, which represents an original result. If the anharmonic part is a polynomial function, the Hamilton function describes an algebraic model which is linear for quadrupole traps. In agreement with the TDVP applied on coherent states, if an anharmonic analytical electric potential is added, then the classical equations of motion turn into coupled nonlinear Hill differential equations. An algorithm results which allows extending the results for any electrical multipole. The classical Hamilton function expressions have been obtained, particularized in case of combined, quadrupole and octupole traps, which is an original result.

The quasienergy spectrum results from the solutions of the Schrödinger equations, expressed as the product between a geometrical (Berry) phase factor and the corresponding symplectic axial or radial coherent states. The results also describe the quantum dynamics of the CM for a system of identical ions, as shown in [4, 12].

The energy function associated to the quantum Hamilton function that characterizes the system is a classical function, whose values are exactly the expected values of the quantum Hamiltonian on coherent states. The classical equations of motion in case of an octupole trap have been obtained, which represents a new result.

Numerical simulations can be used to validate the method suggested in the paper and find the equilibrium configurations for trapped ions or the eigenvalues of normal modes of oscillation. The results in the paper can be also applied to different quantum simulator architectures.

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