Dynamical normal modes for time-dependent Hamiltonians in two dimensions

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We present the theory of time-dependent point transformations to find independent dynamical normal modes for two-dimensional systems subjected to time-dependent control in the limit of small oscillations. The condition that determines if the independent modes can indeed be defined is identified, and a geometrical analogy is put forward. The results explain and unify recent work to design fast operations on trapped ions, needed to implement a scalable quantum-information architecture: Transport, expansions, and the separation of two ions, two-ion phase gates, as well as the rotation of an anisotropic trap for an ion, are treated and shown to be analogous to a mechanical system of two masses connected by springs with time-dependent stiffness.

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I. INTRODUCTION

The small oscillation regime of systems composed by interacting particles is best characterized, and possibly controlled [1], using a decomposition of the dynamics into independent normal modes. For time-independent Hamiltonians, they are concerted and harmonic motions of all particles in the system with frequencies that may be found by diagonalizing the harmonic part of the potential around the equilibrium, using a point canonical transformation that also defines the normal-mode coordinates; see, e.g., Refs. [2–5] in the context of trapped ions. The potential may in principle be also modified externally in a time-dependent manner. Generalizing the normal modes for these time-dependent scenarios is necessary as our ability to drive microscopic or macroscopic systems improves with technological advances; see, e.g., Refs. [6,7]. In this paper we study the possibility to define independent dynamical normal modes in systems described by two-dimensional (2D), time-dependent Hamiltonians. In other words, we study if there is a time-dependent point transformation that defines new coordinates and momenta that behave according to two independent harmonic oscillators. (Note the terminology convention used for time-dependent Hamiltonians: We consider here that coordinates that diagonalize the interaction potential in the quadratic approximation around equilibrium are by definition "normal coordinates." Due to the inertial effects, these normal coordinates may be coupled, even in the quadratic approximation, or independent. The explicit theory in Sec. II and the examples in Sec. III will clarify this point further.) While the question is interesting *per se* and relevant for a broad span of externally controllable physical systems near equilibrium, our main motivation has been the need to understand and possibly improve on recent work to inverse engineer fast and robust operations to drive the motion of trapped ions [8–14].

Trapped ions constitute one of the most developed physical platforms to implement quantum information processing. Since many ions in a single trap are difficult to control, a route towards large-scale computations with many qubits relies on a divide-and-conquer scheme [15,16], where ions are shuttled around in multisegmented Paul traps that hold just a few ions in each processing site. Apart from shuttling, complementary operations such as separating and merging ion chains, rotations, and expansions or compressions may be needed. Coulomb interactions, and controllable external effective potentials determine the motion of the ions and the corresponding Hamiltonians, which can be approximated by quadratic forms near equilibrium. Independent dynamical normal modes for these Hamiltonians are very useful, not only to describe the motion in a simple way but also to inverse engineer the dynamical operations. For operations on one ion in a two-dimensional (2D) potential or on two ions interacting in a one-dimensional (1D) trap [8–14], we noticed that uncoupled dynamical normal modes cannot always be defined. Each case was analyzed separately but a generic understanding of the conditions that determine the coupling and uncoupling of normal-mode coordinates was missing.

This paper presents first in Sec. II a comprehensive theory where the criterion for separability into independent motions by time-dependent point transformations is identified. In Sec. III the theory and criterion are applied to different operations on trapped ion systems. After a final discussion and outlook for future work, Appendix A shows that the general Hamiltonian structure considered describes a mechanical model of two masses connected to walls and to each other by springs with time-dependent stiffness. The treatment in the main text is classical but the results are also valid in the quantum domain, as shown in Appendix B.

II. THE MODEL

Our starting point is a 2D Hamiltonian for two interacting particles moving on a line, with masses m_1 and m_2, (1D) coordinates q_1, q_2, conjugate momenta p_1, p_2, and time-dependent potential $U(q_1,q_2;t)$,

$$H = \frac{p_1^2}{2m_1} + \frac{p_2^2}{2m_2} + U(q_1,q_2;t). \tag{1}$$

The same Hamiltonian structure, with $m = m_1 = m_2$, may also describe one particle moving on a two-dimensional surface with potential U. The first step is to find the equilibrium positions, $q_1^{(0)}$, $q_2^{(0)}$, from the potential minimum given by $\nabla U = 0$, and expand U at that point retaining only quadratic

terms,

$$H = \frac{p_1^2}{2m_1} + \frac{p_2^2}{2m_2} + \frac{1}{2}\sum_{i,j=1}^{2} k_{ij}\big[q_i - q_i^{(0)}(t)\big]\big[q_j - q_j^{(0)}(t)\big]. \quad (2)$$

Because of the generic time dependence of U, the coefficients $k_{ij}(t) = \frac{\partial^2 U}{\partial q_i \partial q_j}|_{q_1^{(0)},q_2^{(0)}}$ and the equilibrium positions $q_i^{(0)}(t)$ may depend on time, but the explicit time dependence will generally be omitted hereafter to avoid a cumbersome notation. The k_{ij} coefficients in Eq. (2) are the elements of the real and symmetric 2×2 matrix K. Being symmetric, it may be parameterized as

$$K = \begin{pmatrix} k+k_1 & -k \\ -k & k+k_2 \end{pmatrix}, \quad (3)$$

where k,k_1,k_2 are generally time dependent. If they are positive, K is a positive matrix (with positive eigenvalues). Defining now the (transpose) vector

$$\psi^T = \big(q_1 - q_1^{(0)}, q_2 - q_2^{(0)}, p_1, p_2\big) \quad (4)$$

and the mass matrix M,

$$M = \begin{pmatrix} m_1 & 0 \\ 0 & m_2 \end{pmatrix}, \quad (5)$$

the Hamiltonian (2) can be written in a compact matrix representation as

$$H = \tfrac{1}{2}\psi^T W \psi, \quad (6)$$

where ψ is the transpose of ψ^T, and W is the 4×4 symmetric matrix formed by K and M^{-1} 2×2 blocks,

$$W = \begin{pmatrix} K & 0 \\ 0 & M^{-1} \end{pmatrix}. \quad (7)$$

Interestingly, the Hamiltonian (6) corresponds as well to a system of two masses connected to walls and to each other by time-dependent spring constants; see Appendix A.

The main goal of this paper is to investigate if there is a point transformation producing new coordinates Q_1, Q_2 and momenta P_1, P_2 such that the corresponding Hamiltonian $\widetilde{H}(Q_1, Q_2, P_1, P_2)$ does not have cross terms and can be separated into independent harmonic motions. We shall see that this is not always possible and we will give the conditions to be satisfied by H in order to successfully separate $\widetilde{H}$ by a time-dependent point transformation. Some alternative treatments when the decomposition fails will also be pointed out.

A. Time-dependent point canonical transformation

Let us consider the general time-dependent (linear) change of coordinates

$$\begin{pmatrix} Q_1 \\ Q_2 \end{pmatrix} = A(t)\begin{pmatrix} q_1 - q_1^{(0)} \\ q_2 - q_2^{(0)} \end{pmatrix}, \quad (8)$$

where $A(t)$ is a 2×2 matrix to be determined, invertible at all times. This transformation is generated by the type-2 generating function [17,18]

$$F_2 = \sum_{i=1}^{2} P_i Q_i(q_1,q_2) = (P_1,P_2)A(t)\begin{pmatrix} q_1 - q_1^{(0)} \\ q_2 - q_2^{(0)} \end{pmatrix}. \quad (9)$$

The momenta transform according to $p_i = \partial_{q_i} F_2$,

$$p_1 = \frac{\partial F_2}{\partial q_1} = a_{11}P_1 + a_{21}P_2,$$

$$p_2 = \frac{\partial F_2}{\partial q_2} = a_{12}P_1 + a_{22}P_2,$$

which can be written in matrix form as

$$\begin{pmatrix} p_1 \\ p_2 \end{pmatrix} = A^T \begin{pmatrix} P_1 \\ P_2 \end{pmatrix}, \quad (10)$$

where A^T denotes the transpose of A. In the four-dimensional representation introduced previously, the canonical transformation of coordinates and momenta is compactly given by

$$\widetilde{\psi} = \begin{pmatrix} A & 0 \\ 0 & A^{-T} \end{pmatrix}\psi, \quad (11)$$

where $\widetilde{\psi}$ is the transpose of $\widetilde{\psi}^T = (Q_1, Q_2, P_1, P_2)$ and $A^{-T} \equiv (A^T)^{-1}$ stands for the inverse of the transpose of A.

B. Inertial effects and effective Hamiltonian

As a consequence of the time dependence of the potential, the coordinate transformation may correspond to a description in a noninertial frame where inertial forces appear. The transformed Hamiltonian in the new coordinates will read $\widetilde{H} = H + \partial_t F_2$, where the last term accounts for inertial effects arising due to the explicit time dependence of F_2,

$$\frac{\partial F_2}{\partial t} = (P_1,P_2)\dot{A}\begin{pmatrix} q_1 - q_1^{(0)} \\ q_2 - q_2^{(0)} \end{pmatrix} - (P_1,P_2)A\begin{pmatrix} \dot{q}_1^{(0)} \\ \dot{q}_2^{(0)} \end{pmatrix}$$

$$= (P_1,P_2)\dot{A}A^{-1}\begin{pmatrix} Q_1 \\ Q_2 \end{pmatrix} - (P_1,P_2)A\begin{pmatrix} \dot{q}_1^{(0)} \\ \dot{q}_2^{(0)} \end{pmatrix}, \quad (12)$$

and the dots denote time derivatives. The inertial effects have two different contributions, a quadratic term proportional to $\dot{A}$ and a linear term proportional to $\dot{q}_i^{(0)}$.

Using the coordinate and momenta transformations (11) and the inertial terms (12), the transformed Hamiltonian in the new coordinates can be written as

$$\widetilde{H} = \frac{1}{2}\tilde{\psi}^T \widetilde{W}\tilde{\psi} - (P_1,P_2)A\begin{pmatrix} \dot{q}_1^{(0)} \\ \dot{q}_2^{(0)} \end{pmatrix}, \quad (13)$$

with

$$\widetilde{W} = \begin{pmatrix} A^{-T}KA^{-1} & (\dot{A}A^{-1})^T \\ \dot{A}A^{-1} & AM^{-1}A^T \end{pmatrix}. \quad (14)$$

Our aim now is to find a transformation matrix A such that $\widetilde{W}$ is a diagonal 4×4 matrix. Since the linear part in the Hamiltonian (13) is already uncoupled, this would define dynamical normal modes [9], evolving independently of each other.

C. Diagonalization of $\widetilde{H}$

To have an uncoupled effective Hamiltonian $\widetilde{H}$ (i.e., a diagonal $\widetilde{W}$), two conditions have to be satisfied: The diagonal blocks in Eq. (14) have to be diagonal 2×2 matrices and the off-diagonal blocks should vanish for all times.

The first one amounts to simultaneously diagonalizing two bilinear forms [17]. As the masses are positive quantities, the square root of the matrix M given in Eq. (5) can be defined as

$$M^{1/2} = \mathrm{diag}(\sqrt{m_1},\sqrt{m_2}). \tag{15}$$

We now define the mass-weighted potential as

$$\widetilde{K} = M^{-1/2} K M^{-1/2}, \tag{16}$$

which is also symmetric since K is symmetric. The explicit expression of the mass-weighted potential $\widetilde{K}$ is

$$\widetilde{K} = M^{-1/2} K M^{-1/2} = \begin{pmatrix} \frac{k+k_1}{m_1} & \frac{-k}{\sqrt{m_1 m_2}} \\ \frac{-k}{\sqrt{m_1 m_2}} & \frac{k+k_2}{m_2} \end{pmatrix}, \tag{17}$$

which, for positive masses, is also positive definite if K is positive. Since $\widetilde{K}$ is in any case symmetric, it can be diagonalized by means of an orthogonal matrix $\mathcal{O}$,

$$\mathcal{O}^T \widetilde{K} \mathcal{O} = \mathrm{diag}\left(\Omega_1^2, \Omega_2^2\right), \tag{18}$$

with

$$\mathcal{O} = \begin{pmatrix} \cos\theta & -\sin\theta \\ \sin\theta & \cos\theta \end{pmatrix}, \tag{19}$$

and where the (generally) time-dependent parameter θ is given by the relation

$$\tan 2\theta = \frac{2k\sqrt{m_1 m_2}}{m_1(k+k_2) - m_2(k+k_1)}. \tag{20}$$

Ω_i^2, the eigenvalues of $\widetilde{K}$, give the time-dependent eigenfrequencies of each normal mode, with explicit expressions

$$\begin{aligned} \Omega_1^2 &= \left(\frac{k+k_1}{m_1}\right)\cos^2\theta + \left(\frac{k+k_2}{m_2}\right)\sin^2\theta \\ &\quad - \frac{k}{\sqrt{m_1 m_2}}\sin 2\theta, \\ \Omega_2^2 &= \left(\frac{k+k_1}{m_1}\right)\sin^2\theta + \left(\frac{k+k_2}{m_2}\right)\cos^2\theta \\ &\quad + \frac{k}{\sqrt{m_1 m_2}}\sin 2\theta, \end{aligned} \tag{21}$$

positive if k, k_1, k_2 are all positive. The modal matrix

$$A = \mathcal{O}^T M^{1/2} = \begin{pmatrix} \sqrt{m_1}\cos\theta & \sqrt{m_2}\sin\theta \\ -\sqrt{m_1}\sin\theta & \sqrt{m_2}\cos\theta \end{pmatrix} \tag{22}$$

diagonalizes simultaneously both the blocks with M^{-1} and K in the main diagonal of Eq. (14) since

$$A^{-T} K A^{-1} = \mathrm{diag}\left(\Omega_1^2, \Omega_2^2\right), \tag{23}$$

$$A M^{-1} A^T = 1. \tag{24}$$

Normal mode coordinates $\{Q_1, Q_2\}$ are defined by the transformation (8) with A given by Eq. (22),

$$\begin{pmatrix} Q_1 \\ Q_2 \end{pmatrix} = \begin{pmatrix} \sqrt{m_1}\cos\theta & \sqrt{m_2}\sin\theta \\ -\sqrt{m_1}\sin\theta & \sqrt{m_2}\cos\theta \end{pmatrix} \begin{pmatrix} q_1 - q_1^{(0)} \\ q_2 - q_2^{(0)} \end{pmatrix}. \tag{25}$$

Note that we have not proved yet if they are uncoupled. They will be independent if the nondiagonal term $\dot{A}A^{-1}$ in Eq. (14) vanishes. With the explicit expression of A in (22) we can calculate the $\dot{A}A^{-1}$ term,

$$\dot{A}A^{-1} = \dot{\theta}\begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}. \tag{26}$$

The effective Hamiltonian becomes

$$\widetilde{H} = \frac{1}{2}\sum_{i=1}^{2}\left(P_i^2 + \Omega_i^2 Q_i^2\right) - (P_1, P_2) A \begin{pmatrix} \dot{q}_1^{(0)} \\ \dot{q}_2^{(0)} \end{pmatrix} - \dot{\theta} L_z, \tag{27}$$

where $L_z = Q_1 P_2 - Q_2 P_1$ has the form of the z component of an angular momentum.

We conclude that if θ does not depend on time, the modes are uncoupled. As we shall see in several examples, some configurations of the matrices K and M lead to $\dot{\theta} = 0$, even if the k, k_1, k_2 are time dependent: For example, $k_1 = c_1 k, k_2 = c_2 k$ with constants c_1, c_2; $k_1 = k_2$ for $m_1 = m_2$; or $k = 0$, with time-dependent k_1 and k_2. If θ is time independent, the new coordinates define indeed independent dynamical normal modes with an uncoupled Hamiltonian

$$\widetilde{H} = \frac{1}{2}\sum_{i=1}^{2}\left(P_i^2 + \Omega_i^2 Q_i^2\right) - (P_1, P_2) A \begin{pmatrix} \dot{q}_1^{(0)} \\ \dot{q}_2^{(0)} \end{pmatrix}. \tag{28}$$

At this point it is customary to perform a momentum shift, so that the new Hamiltonian includes a term linear in coordinates rather than a term linear in momentum. This is done with the generating function

$$F_2 = \sum_{i=1}^{2}(P_i' + P_{0,i}) Q_i,$$

where

$$\begin{pmatrix} P_{0,1} \\ P_{0,2} \end{pmatrix} \equiv A \begin{pmatrix} \dot{q}_1^{(0)} \\ \dot{q}_2^{(0)} \end{pmatrix},$$

which gives for the new momenta and coordinates

$$P_i' = P_i - P_{0,i},$$

$$Q_i' = Q_i,$$

and $\partial_t F_2 = \sum_{i=1}^{2} \dot{P}_{0,i} Q_i'$, so that the transformed Hamiltonian, up to purely time-dependent terms that can be added or subtracted without changing the physics, takes the form of two harmonic oscillators,

$$\widetilde{H}' = \frac{1}{2}\sum_{i=1}^{2}\left[P'^2_i + \Omega_i^2\left(Q'_i + \frac{\dot{P}_{0,i}}{\Omega_i^2}\right)^2\right],$$

whose centers and frequencies may depend on time. While this is the form that has been used to speed up several operations

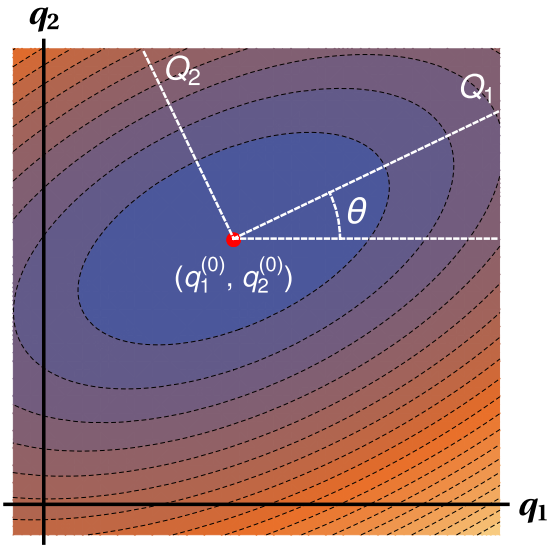

FIG. 1. Schematic representation of isopotential curves of a mass-weighted potential in the two-dimensional configuration space of laboratory-frame coordinates $\{q_1,q_2\}$. These curves are ellipses centered at the moving equilibrium position $(q_1^{(0)},q_2^{(0)})$ with the orientation of the principal axes given by the angle θ. The dynamical normal mode coordinates $\{Q_1,Q_2\}$ are translated from the origin but also rotated by θ.

on trapped ions [8–14], for the discussion of the separability of these systems in Sec. III, it is enough to examine $\widetilde{H}$ so we shall omit the momentum shift transformation.

D. Geometrical interpretation

We have just shown that a condition to define independent modes by a point transformation is that θ (and therefore the transformation A) does not depend on time. What does this parameter represent?

Let us now visualize the mass-weighted symmetric potential $\widetilde{K}$ in Eq. (17) as a matrix defining a quadratic form. Quadratic forms are geometrically represented by conic sections. If $\widetilde{K}$ is positive definite (i.e., with positive eigenvalues), the conic section defined by $\widetilde{K}$ is an ellipse centered at the moving equilibrium position $(q_1^{(0)},q_2^{(0)})$. These ellipses are isopotential curves of the mass-weighted potential $\widetilde{K}$ in the two-dimensional configuration space $\{q_1,q_2\}$; see Fig. 1. The principal axes theorem states that the orthonormal coordinate system where the ellipse is well oriented is given by the orthonormal eigenvectors of $\widetilde{K}$, while the inverse of the square root of its eigenvalues are the radii of the corresponding axes. The orthogonal matrix (19) is formed by the eigenvectors of $\widetilde{K}$,

$$v_1^T = (\cos\theta, \sin\theta),$$
$$v_2^T = (-\sin\theta, \cos\theta).$$

These vectors define the orthonormal coordinate system where the ellipse is well oriented; see Fig. 1. Therefore, the parameter θ gives the orientation of the ellipse. More generally, it gives the orientation of the principal axes if $\widetilde{K}$ is not positive (the engineering of fast dynamics may require that an eigenfrequency becomes transiently an imaginary number [19]). In general for a time-dependent potential, the equilibrium position, the shape (size of principal axes) and orientation (angle θ) will vary in time, but only the rotation of the principal axes couples the normal modes.

III. APPLICATION TO TRAPPED IONS

In this section, we apply the results of the previous sections to systems of two ions in a linear (1D) trap, or one ion in a two-dimensional trap subjected to time-dependent manipulations. In particular, we analyze if independent dynamical normal modes can be defined by time-dependent point transformations. This is a key issue to design and engineer fast and robust protocols for operations such as ion transport [8,9,12], trap expansions or compressions [10], ion splitting [11,20], phase gates [14], or rotations [13]. In many of these works, the simple structure of invariants of motion for harmonic oscillators is used to inverse engineer fast protocols that reach the same populations or even the same states that would result from an adiabatic driving, but in shorter times [21]. Faster-than-adiabatic protocols avoid or mitigate decoherence effects due to noise and perturbations [21]. When the normal-mode oscillators are coupled, the invariants are more involved, which makes the design of fast protocols considerably more challenging than for uncoupled oscillators.

A. Transport and expansions (or compressions) of two interacting trapped ions

Let us consider two singly charged, positive ions in a linear trap at laboratory-frame coordinates q_1 and q_2, coupled via Coulomb interaction and trapped in an external, possibly time-dependent, harmonic potential [9,10]. The external potential can be translated [9] and, in addition, expanded or compressed [10]. The Hamiltonian describing this system is

$$H = \frac{p_1^2}{2m_1} + \frac{p_2^2}{2m_2} + U,$$
$$U = \frac{1}{2}\sum_{i=1}^{2} k(t)[q_i - Q_0(t)]^2 + \frac{C_c}{q_1 - q_2}. \qquad (29)$$

Here, $C_c = \frac{e^2}{4\pi\epsilon_0}$ is the Coulomb constant and $k(t)$ is the common (time-dependent) spring constant that determines the oscillation frequency of each ion ($\omega_i^2 = k/m_i$) in the absence of Coulomb coupling [10]. $Q_0 = Q_0(t)$ defines the position of the minimum of the external potential, i.e., the position of the, possibly moving, trap [9]. We can also set $q_1 > q_2$ because of the strong Coulomb repulsion [8]. If the ions are sufficiently cold, they crystallize around the classical equilibrium positions $q_i^{(0)}$, which are solutions of the set of equations $\frac{\partial U}{\partial q_i} = 0$ for $i = 1,2$,

$$q_1^{(0)} = Q_0 + \left(\frac{C_c}{4k}\right)^{1/3} = Q_0 + \frac{q_0}{2},$$
$$q_2^{(0)} = Q_0 - \left(\frac{C_c}{4k}\right)^{1/3} = Q_0 - \frac{q_0}{2},$$

where $q_0 = q_1^{(0)} - q_2^{(0)} = (2C_c/k)^{1/3}$ is the equilibrium distance between ions.[1] These positions are time dependent but independent of the mass, as we assume that the external potential is due to trap electrodes that interact only with the ionic charge. If we now approximate the coupling potential U by its Taylor expansion truncated to second order in $q_i - q_i^{(0)}$ (small displacements from equilibrium), we end up with a quadratic potential. Therefore, up to a purely time-dependent term, we can approximate the Hamiltonian (29) harmonically as

$$H = \frac{p_1^2}{2m_1} + \frac{p_2^2}{2m_2} + \frac{1}{2}\left(q_1 - q_1^{(0)}, q_2 - q_2^{(0)}\right) K \begin{pmatrix} q_1 - q_1^{(0)} \\ q_2 - q_2^{(0)} \end{pmatrix}, \quad (30)$$

with the K matrix given by

$$K = \begin{pmatrix} 2k & -k \\ -k & 2k \end{pmatrix}.$$

This Hamiltonian corresponds to the case $k_1 = k_2 = k$, so that Eq. (20) gives a constant θ even for a time-dependent k,

$$\tan 2\theta = \frac{\sqrt{m_1 m_2}}{m_1 - m_2}. \quad (31)$$

The normal modes are given by Eq. (25),

$$\begin{pmatrix} Q_1 \\ Q_2 \end{pmatrix} = \begin{pmatrix} \sqrt{m_1}\cos\theta & \sqrt{m_2}\sin\theta \\ -\sqrt{m_1}\sin\theta & \sqrt{m_2}\cos\theta \end{pmatrix} \begin{pmatrix} q_1 - (Q_0 + q_0/2) \\ q_2 - (Q_0 - q_0/2) \end{pmatrix},$$

with θ given by relation (31). These normal modes depend on time through the time-dependent parameters Q_0 and q_0. In these coordinates, the Hamiltonian (30) transforms to the diagonal and uncoupled form (28),

$$\widetilde{H} = \frac{1}{2}\sum_{i=1}^{2}\left(P_i^2 + \Omega_i^2 Q_i^2\right) - (P_1, P_2) A \begin{pmatrix} \dot{Q}_0 + \dot{q}_0/2 \\ \dot{Q}_0 - \dot{q}_0/2 \end{pmatrix}, \quad (32)$$

where

$$\Omega_1^2 = k\left(\frac{2\cos^2\theta}{m_1} + \frac{2\sin^2\theta}{m_2} - \frac{\sin 2\theta}{\sqrt{m_1 m_2}}\right),$$
$$\Omega_2^2 = k\left(\frac{2\sin^2\theta}{m_1} + \frac{2\cos^2\theta}{m_2} + \frac{\sin 2\theta}{\sqrt{m_1 m_2}}\right), \quad (33)$$

which may depend on time because of $k = k(t)$. The inertial effects in the Hamiltonian (32) are in the linear-in-momentum term and are due to the transport ($\dot{Q}_0$ term) and/or expansion or compression of the trap ($\dot{q}_0$ term). Geometrically the center of the ellipses in Fig. 1 can move in the $\{q_1, q_2\}$ plane, and the size may change as well, but the orientation remains constant in time.

[1] As before, we shall generally omit the explicit time dependences of variables such as q_0, k, Q_0, and, later, the mode frequencies Ω_i.

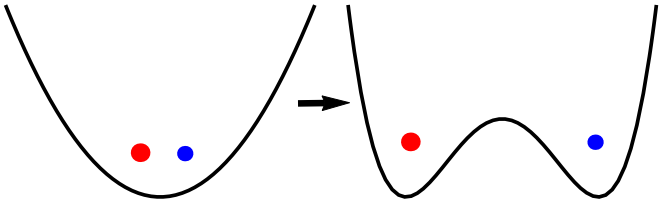

FIG. 2. Scheme of the separation of two ions, from an external harmonic potential to a double well.

B. Separation of two trapped interacting ions

Consider now the problem of separating (or recombining) two interacting trapped ions as in Refs. [11,20]; see Fig. 2. The Hamiltonian of a system of two ions of masses m_1 and m_2 and charge e located at $q_1 > q_2$ in the laboratory frame is

$$H = \frac{p_1^2}{2m_1} + \frac{p_2^2}{2m_2} + U,$$
$$U = \alpha(t)\left(q_1^2 + q_2^2\right) + \beta(t)\left(q_1^4 + q_2^4\right) + \frac{C_c}{q_1 - q_2},$$

where $\alpha(t)$ and $\beta(t)$ are time-dependent functions [11]. Typically $\alpha(0) > 0$, $\beta(0) = 0$, whereas at final time $\beta(t_f) > 0$, $\alpha(t_f) < 0$ to implement an evolution from a harmonic trap to a double well; see Fig. 2.

To set a quadratic (approximate) Hamiltonian we proceed as in the previous subsection: First, we find the equilibrium positions $q_i^{(0)}$ of each ion by minimizing the potential U and then expand the potential U to second order in $q_i - q_i^{(0)}$. If the equilibrium positions are denoted by $q_1^{(0)} = q_0/2$ and $q_2^{(0)} = -q_0/2$, where $q_0 = q_1^{(0)} - q_2^{(0)}$ is the equilibrium distance between ions, this procedure gives the quadratic Hamiltonian

$$H = \frac{p_1^2}{2m_1} + \frac{p_2^2}{2m_2} + \frac{1}{2}\left(q_1 - q_1^{(0)}, q_2 - q_2^{(0)}\right) K \begin{pmatrix} q_1 - q_1^{(0)} \\ q_2 - q_2^{(0)} \end{pmatrix},$$

with a K matrix given by

$$k_1 = k_2 = 2\alpha + 3\beta q_0^2 = k_0,$$
$$k = \frac{2C_c}{q_0^3},$$

and where q_0 is the solution of the quintic equation [11,20]

$$\beta q_0^5 + 2\alpha q_0^3 - 2C_c = 0. \quad (34)$$

In this case

$$\tan 2\theta = \frac{\sqrt{m_1 m_2}}{m_1 - m_2}\left(\frac{4C_c}{2\alpha q_0^3 + 3\beta q_0^5 + 2C_c}\right), \quad (35)$$

which, in general, depends on time. In principle, there are two ways to end up with a time-independent θ for time dependent α and β:

(1) Equal masses, $m_1 = m_2$, for which $\theta = \pm\pi/4$ regardless of the time dependence of α and β [11].

(2) α and β linked by

$$\frac{\beta^3}{\alpha^5} = \text{constant}, \tag{36}$$

regardless of the masses. This implies that the products βq_0^5 and αq_0^3 are constants. The particular case $\beta = 0$ corresponds to the one considered in the previous subsection (transport and expansions). The case $\beta \neq 0$ is interesting as it allows us to separate or approach the two ions by decreasing or increasing $\alpha < 0$ and $\beta > 0$ according to Eq. (36), i.e., in a double-well confining potential throughout the process.

C. Phase gates

A phase gate can be implemented by applying well-designed time-dependent forces that depend on the internal states of the two ions in a linear trap [14]. The external harmonic trap for each ion has a fixed spring constant k_0. For a particular spin configuration the Hamiltonian becomes

$$H = \frac{p_1^2}{2m_1} + \frac{p_2^2}{2m_2} + \frac{1}{2}k_0\left(q_1^2 + q_2^2\right) + \frac{C_c}{q_1 - q_2} + F_1(t)q_1 + F_2(t)q_2. \tag{37}$$

Equilibrium positions and the equilibrium distance between the ions are

$$q_1^{(0)} = \frac{B - 2k_0^2\Delta(F_2 + 2F_1)}{6k_0^3\Delta},$$

$$q_2^{(0)} = \frac{-B - 2k_0^2\Delta(F_1 + 2F_2)}{6k_0^3\Delta},$$

$$q_0 = q_1^{(0)} - q_2^{(0)} = \frac{2B - 2k_0^2\Delta(F_1 + F_2)}{6k_0^3\Delta},$$

where

$$B = (F_1 - F_2)^2k_0^4 + \Delta^2,$$

$$\Delta = \Big\{ -(F_1 - F_2)^3k_0^6 + 27C_ck_0^8 + 3\sqrt{3C_ck_0^{14}\left[-2(F_1 - F_2)^3 + 27C_ck_0^2\right]}\Big\}^{1/3}.$$

This leads to a K matrix with

$$k = \frac{2C_c}{q_0^3}, \quad k_1 = k_2 = k_0,$$

so that

$$\tan 2\theta = \frac{\sqrt{m_1m_2}}{m_1 - m_2}\frac{4C_c}{k_0q_0^3 + 2C_c}.$$

The angle θ is in general time dependent, but it becomes constant in some cases, specifically for $m_1 = m_2$, and also for $F_1 = F_2$. This latter case, in fact, reduces to the transport of two ions considered before. For different masses and forces the ellipsoid rotates so that Q_1, Q_2 are coupled. A way out, if the forces are small so that the linear term in Eq. (37) may be considered a perturbation, is to define the modes for the zeroth-order Hamiltonian [22]

$$H_0 = \frac{p_1^2}{2m_1} + \frac{p_2^2}{2m_2} + \frac{1}{2}k_0\left(q_1^2 + q_2^2\right) + \frac{C_c}{q_1 - q_2}.$$

The zeroth-order modes, $Q_1(F_j = 0)$, $Q_2(F_j = 0)$, $j = 1,2$, are of course uncoupled since all coefficients in H_0 are time independent. H_0 may thus be easily diagonalized. Specifically, all the K matrix coefficients become equal, $\tan 2\theta = \frac{\sqrt{m_1m_2}}{m_1 - m_2}$, and the equilibrium positions simplify to the constant values $\pm[\frac{C_c}{4k_0}]^{1/3}$. The inverse transformation of Eq. (25) for these zeroth-order modes,

$$\begin{pmatrix} q_1 \\ q_2 \end{pmatrix} = \begin{pmatrix} q_1^{(0)} \\ q_2^{(0)} \end{pmatrix}_{F_j=0} + A^{-1}_{F_j=0}\begin{pmatrix} Q_1 \\ Q_2 \end{pmatrix}_{F_j=0},$$

enables us to write the perturbative linear terms in H in terms of the uncoupled modes, so that $\widetilde{H}$ is approximated as a sum of two uncoupled Hamiltonians [14,22].

D. Anisotropic harmonic oscillator in 2D with rotation

Consider now a single particle of mass m trapped in a 2D anisotropic harmonic oscillator which is rotating around the z axis with angular velocity $\dot{\varphi}$ [23]. Let us denote by $q_1 = x$ and $q_2 = y$ the laboratory frame coordinates of the ion, and by

$$\tilde{q}_1(t) = q_1\cos\varphi(t) + q_2\sin\varphi(t),$$

$$\tilde{q}_2(t) = -q_1\sin\varphi(t) + q_2\cos\varphi(t), \tag{38}$$

the coordinates in the rotating frame. The Hamiltonian in the laboratory frame is given by

$$H = \frac{p_1^2}{2m} + \frac{p_2^2}{2m} + \frac{1}{2}m\sum_{i=1}^{2}\omega_i^2\tilde{q}_i(q_1,q_2;t)^2,$$

where $\omega_1 \neq \omega_2$ are the angular frequencies along the rotating principal axes. (For the trivial isotropic case $\omega_1 = \omega_2$ the Hamiltonian is already uncoupled in the laboratory frame.) H can be written as

$$H = \frac{p_1^2}{2m} + \frac{p_2^2}{2m} + \frac{1}{2}(q_1,q_2)K\begin{pmatrix} q_1 \\ q_2 \end{pmatrix}, \tag{39}$$

with the K matrix elements given by

$$k_1 = m\left(\omega_1^2\cos^2\varphi + \omega_2^2\sin^2\varphi\right) - k,$$

$$k_2 = m\left(\omega_1^2\sin^2\varphi + \omega_2^2\cos^2\varphi\right) - k,$$

$$k = -\frac{m}{2}\left(\omega_1^2 - \omega_2^2\right)\sin 2\varphi.$$

Unlike the previous operations, there is no need to make the harmonic approximation around the equilibrium since H is already quadratic. Moreover, $q_1^{(0)} = q_2^{(0)} = 0$ and, quite simply, $\theta = \varphi$. The Hamiltonian $\tilde{H}$ takes the form in Eq. (27) without the linear term and with $\Omega_i = \omega_i$, and $Q_i = \sqrt{m}\tilde{q}_i$; i.e., the normal-mode coordinates are the (mass-weighted) rotating coordinates in Eq. (38), coupled by the angular momentum term $-\dot{\theta}L_z$. We conclude that the 2D anisotropic problem is not separable by means of a linear point transformation of coordinates.

Making use of an additional physical interaction, it is possible to cancel the coupling term so that the resulting Hamiltonian is diagonal. Specifically, if the particle is an ion of (positive) charge e, a homogeneous magnetic field $-B\hat{z}$ introduces, in the rotating frame, the diamagnetic and

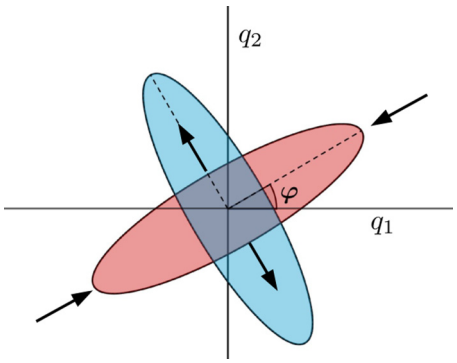

FIG. 3. Compression and expansion along the nonrotating principal axes of a 2D anisotropic oscillator amounts to a $\pi/2$ rotation of the potential.

paramagnetic terms, see, e.g., Ref. [24],

$$\tfrac{1}{2}\omega_L^2\left(Q_1^2+Q_2^2\right)+\omega_L L_z,$$

where the Larmor frequency is $\omega_L = eB/(2m)$. Adjusting the magnetic field to exactly cancel $-\dot{\theta}L_z$ with $\omega_L = \dot{\theta}$, provides an uncoupled normal-mode Hamiltonian with time-dependent frequencies $[\omega_i^2+\omega_L^2]^{1/2}$. Note that the harmonic 2D potential complemented by a confining term in the z direction cannot be purely electrostatic as it would not obey Laplace's equation [23]. It could, however, be created by other means, for example, as an effective pondermotive potential.

1. Compressions and expansions

We have pointed out before that $k = 0$, with k_1 and k_2 time dependent, leads to constant θ and independent modes. For a single particle in a harmonic potential, this corresponds to time-dependent frequencies (expansions and compressions) along nonrotating principal axes of the potential. Specific orthogonal compressions and expansions where the two normal-mode frequencies interchange amount at final time to a $\frac{\pi}{2}$ rotation of the potential, see Fig. 3, although the process itself is different from a true rotation. Slow adiabatic expansion and compression processes would connect initial and final excited energy levels differently from a true rotation, which may be important for inverse engineering operations. During the manipulation of the frequencies the levels cross, so that their energy ordering changes. Take, for example, the initial states with vibrational quantum numbers 01 and 10 for the principal directions 1 and 2 and such that $\omega_1 < \omega_2$. Then the energies satisfy initially $E_{01} > E_{10}$. If the values of the frequencies are interchanged along the process, the energies also switch, $E_{10} > E_{10}$. On the contrary, a slow true rotation does not produce crossings and energy reordering.

IV. DISCUSSION

Motivated by the need to inverse engineer the dynamics of trapped ions and other systems in the small oscillations regime, we have studied the possibility to define, via linear point transformations, independent dynamical normal modes for two-dimensional systems under time-dependent external control. Whereas the analysis of further dimensions is certainly worthwhile, two dimensions are already relevant, as they suffice to describe pairs of ions in linear traps, and universal quantum computing may be achieved by combining operations on one and two qubits. We also expect that the results found here may set a useful guide for further dimensions. The condition that determines the coupling of the modes turns out to be the rotation of the harmonic potential in the (laboratory) 2D coordinate space. Nonrotating potentials lead to uncoupled dynamical modes. Different examples have been analyzed and in some of them ways to avoid the coupling have been pointed out: by a specific design of the time dependence of the control parameters in separation operations or by adding compensating terms in the Hamiltonian in rotations or perturbatively in phase gates. Point transformations are the ones used for time-independent normal-mode analysis, so they are a natural choice. Moreover, they are easy to understand, visualize, and implement. More general (mixed) canonical transformations have not been considered in this paper, but they are in principle possible [25–30] and will be discussed elsewhere. Generically their physical meaning, definition, and practical use become more involved, so only simplified potential configurations and dynamics are typically worked out explicitly [25–30].

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APPENDIX A: DERIVATION OF THE HAMILTONIAN OF THE SPRING SYSTEM

In this Appendix we find the Hamiltonian describing the dynamics of two masses connected by springs as illustrated in Fig. 4. The three springs are assumed to have zero natural length but time-dependent spring constants. If q_i is the laboratory frame coordinate of m_i measured from the fixed left wall, the Hamiltonian is given by

$$H = \frac{p_1^2}{2m_1}+\frac{p_2^2}{2m_2}+U,$$

$$U = \frac{1}{2}k_1q_1^2+\frac{1}{2}k_2(d-q_2)^2+\frac{1}{2}k(q_2-q_1)^2,$$

where p_i is the conjugate momentum of the coordinate q_i. By solving the set of equations $\partial_{q_i}U = 0$ for $i = 1,2$ we find the

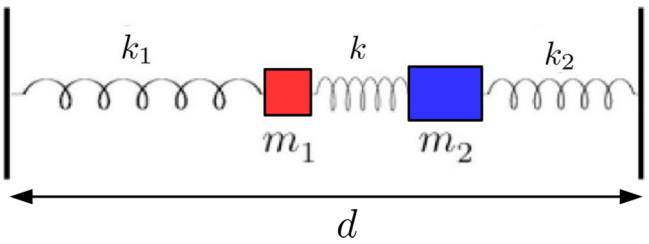

FIG. 4. Mechanical system of two masses connected to each other and to the walls by springs with time-dependent spring constants. This system is found to be mathematically equivalent to many of the trapped ions systems considered throughout the text.

equilibrium positions of the two connected masses at

$$q_1^{(0)} = q_0 \frac{k}{k_1},$$

$$q_2^{(0)} = q_1^{(0)} + q_0,$$

where $q_0 = q_2^{(0)} - q_1^{(0)}$, the equilibrium distance between masses, is given by

$$q_0 = d\left[\frac{k_1 k_2}{k_1 k_2 + k(k_1 + k_2)}\right].$$

The equilibrium positions are generally moving; they depend on time because of the time dependence of k, k_1, and k_2. We can now expand the coupling potential U around its equilibrium position (small oscillations), and up to a purely time-dependent function, we have

$$U = \frac{1}{2}(q_1 - q_1^{(0)}, q_2 - q_2^{(0)}) \begin{pmatrix} k_1 + k & -k \\ -k & k_2 + k \end{pmatrix} \begin{pmatrix} q_1 - q_1^{(0)} \\ q_2 - q_2^{(0)} \end{pmatrix},$$

where the $q_i - q_i^{(0)}$ measure the displacement of mass m_i from its (moving) equilibrium position. The full Hamiltonian then may be written exactly as in Eq. (6).

APPENDIX B: QUANTUM TREATMENT

The results in the main text regarding the form of the Hamiltonians and transformations can be used directly in quantum mechanical systems. The starting point is the 2D time-dependent Schrödinger equation

$$i\hbar \partial_t \psi(q_1, q_2; t) = H(q_1, q_2; t)\psi(q_1, q_2; t), \tag{B1}$$

with $H(q_1, q_2; t)$ given in Eq. (2). Let us now consider the use of the new coordinates (8) and define

$$\Psi = \Psi(Q_1, Q_2; t) \equiv \psi[q_1(Q_1, Q_2; t), q_2(Q_1, Q_2; t); t]. \tag{B2}$$

We now calculate the time derivative of the transformed wave function taking into account the time dependences separately and applying the chain rule,

$$\begin{aligned} i\hbar \partial_t \Psi &= i\hbar \partial_t \psi[q_1(Q_1, Q_2; t), q_2(Q_1, Q_2; t); t] \\ &= i\hbar \left[\partial_t + \partial_t q_1 \partial_{q_1} + \partial_t q_2 \partial_{q_2}\right]\Psi \\ &= \left[H(Q_1, Q_2) - (p_1, p_2)\begin{pmatrix} \partial_t q_1 \\ \partial_t q_2 \end{pmatrix}\right]\Psi, \end{aligned} \tag{B3}$$

with $p_j = -i\hbar \partial_{q_j}$. The first term is just the transformed Hamiltonian, i.e., the original Hamiltonian written in the new coordinates with the usual definition $P_j = -i\hbar \partial_{Q_j}$, and the second term is an inertial contribution due to the time dependence of the transformation. It is now clear that the effective Hamiltonian is

$$\widetilde{H}(Q_1, Q_2) = H(Q_1, Q_2) - (P_1, P_2) A \begin{pmatrix} \partial_t q_1 \\ \partial_t q_2 \end{pmatrix}, \tag{B4}$$

where relation (10) has been used to write the old momenta in terms of the new ones. The explicit time derivative of the q_i coordinates in (B4) can be calculated directly by inverting transformation (8),

$$\begin{pmatrix} \partial_t q_1 \\ \partial_t q_2 \end{pmatrix} = \begin{pmatrix} \dot{q}_1^{(0)} \\ \dot{q}_2^{(0)} \end{pmatrix} + \partial_t (A^{-1}) \begin{pmatrix} Q_1 \\ Q_2 \end{pmatrix}, \tag{B5}$$

which leads finally to an effective Hamiltonian

$$\begin{aligned} \widetilde{H} &= H - (P_1, P_2) A \begin{pmatrix} \dot{q}_1^{(0)} \\ \dot{q}_2^{(0)} \end{pmatrix} - (P_1, P_2) A \partial_t (A^{-1}) \begin{pmatrix} Q_1 \\ Q_2 \end{pmatrix} \\ &= H - (P_1, P_2) A \begin{pmatrix} \dot{q}_1^{(0)} \\ \dot{q}_2^{(0)} \end{pmatrix} - \dot{\theta}(Q_1 P_2 - Q_2 P_1), \end{aligned} \tag{B6}$$

where, for writing the last term, we have used the relation

$$A \partial_t (A^{-1}) = \dot{\theta} \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}. \tag{B7}$$

The effective Hamiltonian when using transformed coordinates thus takes exactly the same form as in classical mechanics, Eq. (27).

[1] J. I. Cirac and P. Zoller, Phys. Rev. Lett. **74**, 4091 (1995).
[2] A. M. Steane, Appl. Phys. B **64**, 623 (1997).
[3] D. V. F. James, Appl. Phys. B **66**, 181 (1998).
[4] G. Morigi and H. Walther, Eur. Phys. J. D **13**, 261 (2001).
[5] J. P. Home, D. Hanneke, J. D. Jost, D. Leibfried, and D. J. Wineland, New J. Phys. **13**, 073026 (2011).
[6] H. Landa, M. Drewsen, B. Reznik, and A. Retzker, New J. Phys. **14**, 093023 (2012).
[7] H. Landa, M. Drewsen, B. Reznik, and A. Retzker, J. Phys. A: Math. Theor. **45**, 455305 (2012).
[8] M. Palmero, E. Torrontegui, D. Guéry-Odelin, and J. G. Muga, Phys. Rev. A **88**, 053423 (2013).
[9] M. Palmero, R. Bowler, J. P. Gaebler, D. Leibfried, and J. G. Muga, Phys. Rev. A **90**, 053408 (2014).
[10] M. Palmero, S. Martínez-Garaot, J. Alonso, J. P. Home, and J. G. Muga, Phys. Rev. A **91**, 053411 (2015).
[11] M. Palmero, S. Martínez-Garaot, U. G. Poschinger, A. Ruschhaupt, and J. G. Muga, New J. Phys. **17**, 093031 (2015).
[12] X. J. Lu, M. Palmero, A. Ruschhaupt, X. Chen, and J. G. Muga, Phys. Scr. **90**, 074038 (2015).
[13] M. Palmero, S. Wang, D. Guéry-Odelin, Jr-Shin Li, and J. G. Muga, New J. Phys. **18**, 043014 (2016).
[14] M. Palmero, S. Martínez-Garaot, D. Leibfried, D. J. Wineland, and J. G. Muga, Phys. Rev. A **95**, 022328 (2017).
[15] D. J. Wineland, C. Monroe, W. M. Itano, D. Leibfried, B. E. King, and D. M. Meekhof, J. Res. Natl. Inst. Stand. Technol. **103**, 259 (1998).

[16] D. Kielpinski, C. Monroe, and D. J. Wineland, Nature (London) **417**, 709 (2002).
[17] H. Goldstein, C. Poole, and J. Safko, *Classical Mechanics*, 3rd ed. (Addison-Wesley, Reading, MA, 2001).
[18] W. Dittrich and M. Reuter, *Classical and Quantum Dynamics* (Springer, Berlin, 2001).
[19] X. Chen, A. Ruschhaupt, S. Schmidt, A. del Campo, D. Guéry-Odelin, and J. G. Muga, Phys. Rev. Lett. **104**, 063002 (2010).
[20] J. P. Home and A. M. Steane, Quantum Inf. Comput. **6**, 289 (2006).
[21] E. Torrontegui, S. Ibañez, S. Martínez-Garaot, M. Modugno, A. del Campo, D. Guéry-Odelin, A. Ruschhaupt, X. Chen, and J. G. Muga, Adv. Atom. Mol. Opt. Phys. **62**, 117 (2013).
[22] J. J. García-Ripoll, P. Zoller, and J. I. Cirac, Phys. Rev. A **71**, 062309 (2005).
[23] S. Masuda and S. A. Rice, J. Phys. Chem. B **119**, 11079 (2015).
[24] M. G. Calkin, *Lagrangian and Hamiltonian Mechanics: Solutions to the Exercises* (World Scientific, Singapore, 1999).
[25] V. V. Dodonov and V. I. Manko, in *Proceedings of the P. N. Lebedev Physical Institute*, Vol. 183, edited by M. A. Markov (Nova Science, Commack, NY, 1987).
[26] F. Leyvraz, V. I. Manko, and T. H. Seligman, Phys. Lett. A **210**, 26 (1996).
[27] J.-Y. Ji and J. Hong, J. Phys. A: Math. Gen. **31**, L689 (1998).
[28] X.-W. Xu, J. Phys. A: Math. Gen. **33**, 2447 (2000).
[29] M. S. Abdalla and P. G. Leach, J. Phys. A: Math. Gen. **38**, 881 (2005).
[30] S. Menouar, M. Maamache, and J. R. Choi, Ann. Phys. **325**, 1708 (2010).