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A dynamical systems approach to Bohmian trajectories in a 2D harmonic oscillator

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Abstract

Vortices are known to play a key role in the dynamics of the quantum trajectories defined within the framework of the de Broglie–Bohm formalism of quantum mechanics. It has been rigorously proved that the motion of a vortex in the associated velocity field can induce chaos in these trajectories, and numerical studies have explored the rich variety of behaviors that due to their influence can be observed. In this paper, we go one step further and show how the theory of dynamical systems can be used to construct a general and systematic classification of such dynamical behaviors. This should contribute to establish some firm grounds on which the studies on the intrinsic stochasticity of Bohm’s quantum trajectories can be based. An application to the two-dimensional isotropic harmonic oscillator is presented as an illustration.

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1. Introduction

Some interpretational difficulties [1] with the standard version [2] led David Bohm to develop in the 1950s [3] an alternative formulation of quantum mechanics. Despite initial criticisms, this theory has recently received much attention [4, 5], having experienced in the past few years an important revitalization, supported by a new computationally oriented point of view. In this way, many interesting practical applications, including the analysis of the tunneling mechanism [6–8], scattering processes [9–11] or the classical-quantum correspondence [12, 13], just to name a few, have been revisited using this novel point of view. Also,

the chaotic properties of these trajectories [14–18], or more fundamental issues, such as the extension to quantum field theory [19], or the dynamical origin of Born's probability rule [20] (one of the most fundamental cornerstones of the quantum theory), have been addressed within this framework.

Most interesting in Bohmian mechanics is the fact that this theory is based on quantum trajectories, 'piloted' by the de Broglie's wave which creates a (quantum) potential term additional to the physical one derived from the actual forces existing in the system [3]. This term brings into the theory interpretative capabilities in terms of intuitive concepts and ideas, which are naturally deduced due to fact that quantum trajectories provide causal connections between physical events well defined in configuration and time. Once these ideas have been established as the basis of many numerical studies, it becomes, in our opinion, of great importance to provide firm dynamical grounds that can support the arguments based on quantum trajectories. For example, it has been recently discussed that the chaotic properties of quantum trajectories are critical for a deep understanding of Born's probability quantum postulate, considering it as an emergent property [20]. Unfortunately very little progress, i.e. rigorous formally proved mathematical results, has taken place along this line due to the lack of a solid theory that can foster this possibility. Moreover, there are cases in the literature clearly demonstrating the dangers of not proceeding in this way. One example can be found in [21], where a chaotic character was ascribed to quantum trajectories for the quartic potential, supporting the argument solely on the fact that numerically computed neighboring pairs separate exponentially. This analysis was clearly done in a way in which the relative importance of the quantum effects could not be gauged. Something even worse happened with the results reported in [22], that were subsequently proved to be wrong in a careful analysis of the trajectories [23].

Recently, some of the authors have made in [15–17] what we consider a relevant advance along the line proposed in this paper, by considering the relationship between the eventual chaotic nature of quantum trajectories and the vortices existing in the associated velocity field which is given by the quantum potential, a possibility that had been pointed out previously by Frisk [14]. Vortices have always attracted the interest of scientists from many different fields. They are associated with singularities at which certain mathematical properties become infinity or abruptly change, and play a central role to explain many interesting phenomena in both classical and quantum physics [25]. In [15–17] it was shown that quantum trajectories are, in general, intrinsically chaotic, being the motion of the velocity field vortices a sufficient mechanism to induce this complexity [15]. In this way, the presence of a single moving vortex, in an otherwise classically integrable system, is enough to make quantum trajectories chaotic. When two or few vortices exist, the interaction among them may end up in the annihilation or creation of them in pairs with opposite vorticities. This phenomenon makes the size of the regular regions in phase space grow as vortices disappear [17]. Finally, it has been shown that when a great number of vortices are present the previous conclusions also hold, and they statistically combine in such a way that they can be related to a suitably defined Lyapunov exponent, as a global numerical indicator of chaos in the quantum trajectories [16]. Summarizing, this makes chaos the general dynamical scenario for quantum trajectories, and this is due to the existence and motion of the vortices of the associated velocity field.

In this paper, we extend and rigorously justify the numerical results in [15–17] concerning the behavior of quantum trajectories and its structure by presenting the general analysis of a particular problem of general interest, namely a two-dimensional harmonic oscillator, where chaos does not arise from classical reasons. In this way, we provide a systematic classification of all possible dynamical behaviors of the existing quantum trajectories, based on the application of dynamical systems theory [24]. This classification provides a complete

‘road map’ which makes possible a deep understanding, put on firm grounds, of the dynamical structure for the problem being addressed.

2. Bohmian mechanics and quantum trajectories

The Bohmian mechanics formalism of quantum trajectories starts from the suggestion made by Madelung of writing the wavefunction in polar form

$$\psi(r, t) = R(r, t) e^{iS(r, t)},$$

where $R^2 = \bar{\psi}\psi$ and $S = (\ln \psi - \ln \bar{\psi})/(2i)$ are two real functions of position and time respectively. For convenience, we set $\hbar = 1$ throughout the paper, and consider a particle of unit mass. Substitution of this expression into the time-dependent Schrödinger equation allows us to recast the quantum theory into a ‘hydrodynamical’ form [5], which is governed by

$$\frac{\partial R^2}{\partial t} = -\nabla \cdot (R^2 \nabla S), \quad (1)$$

$$\frac{\partial S}{\partial t} = -\frac{(\nabla S)^2}{2} - V - \frac{1}{2} \frac{\nabla^2 R}{R}, \quad (2)$$

which are the continuity and the ‘quantum’ Hamilton–Jacobi equations, respectively. The qualifying term in the last expression is customarily included since this equation contains an extra non-local contribution (determined by the quantum state), $Q = \frac{1}{2} \nabla^2 R/R$, called the ‘quantum’ potential. Together with V , this additional term determines the total force acting on the system, and it is responsible for the so-called quantum effects in the dynamics of the system.

Similarly to what happens in the standard Hamilton–Jacobi theory, equations (1) and (2) allow us to define, for spinless particles, quantum trajectories by integration of the differential equation system: $\dot{r} = -\nabla V(r) - \nabla Q(r)$. Alternatively, one can consider the velocity vector field

$$X_\psi = \nabla S = \frac{i}{2} \frac{\psi \nabla \bar{\psi} - \bar{\psi} \nabla \psi}{|\psi|^2}. \quad (3)$$

Note that, in general, this Bohmian vector field is not Hamiltonian, but it may nevertheless have some interesting properties. In particular, for the example considered in this paper it will be shown that it is time-reversible, this symmetry allowing the study of its dynamics in a systematic way.

Let us recall that a system, $\dot{r} = X(r, t)$, is time-reversible if there exists an involution, $r = \Theta(s)$, that is a change of variables satisfying $\Theta^2 = \text{Id}$ and $\Theta \neq \text{Id}$, such that the new system results in $\dot{s} = D\Theta^{-1}(s)X(\Theta(s), t) = -X(s, t)$. One of the dynamical consequences of reversibility is that if $r(t)$ is a solution, then so it is $\Theta(r(-t))$. This fact introduces symmetries in the system giving rise to relevant dynamical constraints. For example, let us assume that $\Theta(x, y) = (x, -y)$ is a time-reversible symmetry (see figure 1). Then any solution $r(t) = (x(t), y(t))$ defines another solution given by $(x(-t), -y(-t))$. Let us remark that this fact constraints the system dynamics since if, for example, $r(t)$ crosses the symmetry axis ($y = 0$ is invariant under Θ), then the two solutions must coincide.

We conclude this section by stressing that time-reversible systems generated a lot of interest during the 1980s due to the fact that they exhibit most of the properties of Hamiltonian systems (see [26–28]). In particular, this type of systems can have quasi-periodic tori which

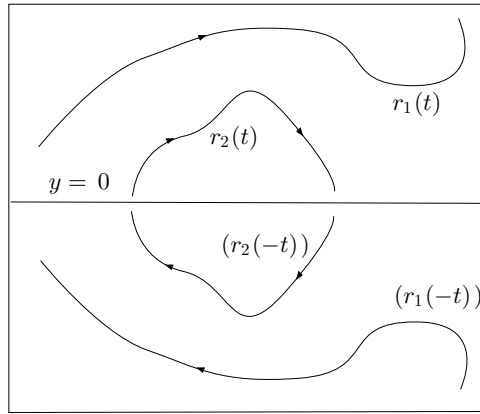


Figure 1. Illustration of the dynamical consequences of a time-reversible symmetry.

are invariant under both the flow and the involution Θ . That is, KAM theory fully applies in this context. Furthermore, some interesting results concerning the splitting of separatrices have been developed successfully for time-reversible systems [29], providing powerful tools for the study of homoclinic and heteroclinic chaos.

3. Model and canonical form

The system that we choose to study is the two-dimensional isotropic harmonic oscillator. Without loss of generality, the corresponding Hamiltonian operator for $r = (x, y)$ can be written in the form

$$\hat{H}(x, y) = -\frac{1}{2} \left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} \right) + \frac{1}{2} (x^2 + y^2).$$

In this paper, we consider the particular combination of eigenstates: $\varphi_{0,0} = 1/\sqrt{\pi}$ with energy 1, and $\varphi_{1,0} = 2x/\sqrt{2\pi}$, $\varphi_{0,1} = 2y/\sqrt{2\pi}$ with energy 2. It can be immediately checked that the time evolution of the resulting wavefunction is given by

$$\psi = \left(\frac{\mathcal{A} e^{-it}}{\sqrt{\pi}} + \frac{2x\mathcal{B} e^{-2it}}{\sqrt{2\pi}} + \frac{2y\mathcal{C} e^{-2it}}{\sqrt{2\pi}} \right) e^{-\frac{1}{2}(x^2+y^2)}, \quad (4)$$

where⁴ $\mathcal{A} = A + iD$, $\mathcal{B} = B + iE$ and $\mathcal{C} = F + iG$, subject to the usual normalization condition $|\mathcal{A}|^2 + |\mathcal{B}|^2 + |\mathcal{C}|^2 = 1$. In addition, we further assume the condition $BC \neq EF$ in order to ensure the existence of a unique vortex in the velocity field at any time. Accordingly, the quantum trajectories associated with (4) are solutions of the system of differential equations:

$$\dot{x} = \frac{-2(BC - EF)y - \sqrt{2}(BD - AE) \cos t - \sqrt{2}(AB + DE) \sin t}{V(x, y, t)}, \quad (5)$$

$$\dot{y} = \frac{2(BC - EF)x + \sqrt{2}(AC - DF) \cos t - \sqrt{2}(DC + AF) \sin t}{V(x, y, t)}, \quad (6)$$

⁴ The choice of notation for the real and imaginary parts of $\mathcal{C}$ may look arbitrary at this point, but it makes simpler the notation for the canonical form introduced in the next section.

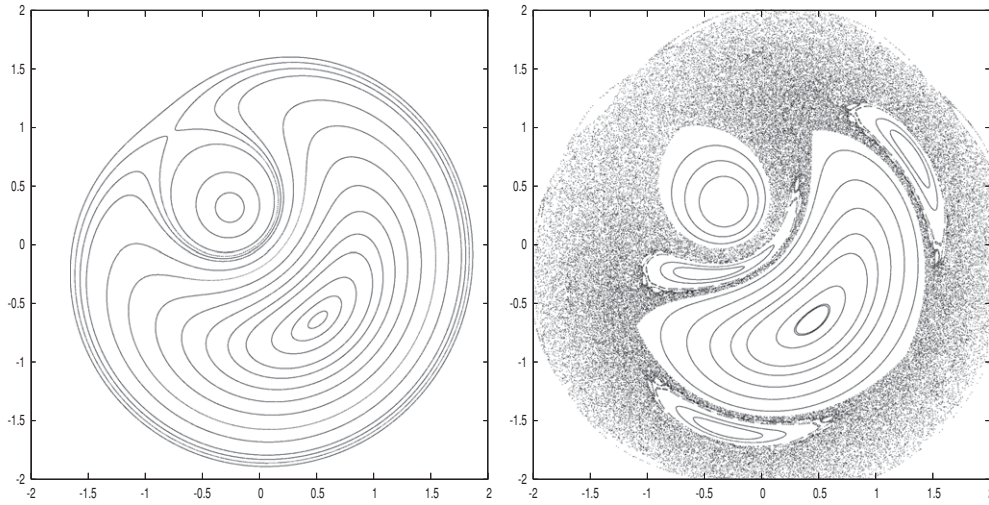


Figure 2. Stroboscopic 2π -periodic sections for the quantum trajectories generated by equations (5) and (6) for different values of the normalized constants. Left plot: $A = 0.37$, $D = -0.02$, $B = C = 0.44$ and $E = -F$. Right plot: $A = 0.4$, $D = -0.018$, $B = 0.37$ and $C = E = 0.49$.

where

$$V(x, y, t) = 2(B^2 + E^2)x^2 + 2(C^2 + F^2)y^2 + 4(BF + EC)xy + D^2 + A^2 \\ + 2\sqrt{2}((AB + DE)\cos t + (AE - DB)\sin t)x \\ + 2\sqrt{2}((DC + AF)\cos t + (AC - DF)\sin t)y.$$

To integrate this equation a 7/8th-order Runge–Kutta–Fehlberg method has been used. Moreover, since the vector field is periodic, the dynamics can be well monitored by using stroboscopic sections. In particular, we plot the solution $(x(t), y(t))$ at times $t = 2\pi n$ for $n = 1, 2, \dots, 10^4$ and for several initial conditions.

In figure 2 we show the results of two such stroboscopic sections. As can be seen the left plot corresponds to completely integrable motions, whereas the right one to sizeable chaotic zones coexisting with stability islands, this strongly suggesting the applicability of the KAM scenario. However, our vector field is neither Hamiltonian nor time-reversible, and then the KAM theory does not directly apply to this case. However, we will show how a suitable change of variables can be performed that unveils a time-reversible symmetry existing in our vector field. For this purpose, we first recall that the structure of gradient vector fields is preserved under orthogonal transformations. In this way, if we consider the transformation $r = Ms$, with $M^T = M^{-1}$, applied to $\dot{r} = \nabla S(r, t)$, we have that $\dot{s} = \nabla \tilde{S}(s, t)$, being $\tilde{S}(s, t) = S(Ms, t)$. In other words, any orthogonal transformation can be performed on the wavefunction instead of on the vector field.

Lemma 3.1. *If equation (4) satisfies the non-degeneracy condition $BC \neq EF$, then there exist an orthogonal transformation and a time shift, such that the wavefunction takes the form*

$$\psi = \left(\frac{\hat{A} e^{-it}}{\sqrt{\pi}} + \frac{2x \hat{B} e^{-2it}}{\sqrt{2\pi}} + \frac{2yi \hat{C} e^{-2it}}{\sqrt{2\pi}} \right) e^{-\frac{1}{2}(x^2+y^2)}, \quad (7)$$

where $\hat{A}, \hat{B}, \hat{C} \in \mathbb{R}$, $\hat{B} > 0$, $\hat{C} \neq 0$, satisfy $\hat{A}^2 + \hat{B}^2 + \hat{C}^2 = 1$.

Table 1. Wavefunction coefficients in the canonical model corresponding to the results of figure 2. Hats have been omitted as discussed in the text.

	Left plot	Right plot
A	0.370 540 146 272 978	0.400 404 795 176 082
B	0.656 772 411 113 622	0.705 788 460 189 184
C	0.656 772 411 113 622	0.584 413 081 188 110

We will refer to the wavefunction (7) as the canonical form of (4), and the rest of the paper is devoted to the study of this case. For this reason, the hat in the coefficients will be omitted, since it is understood that $D = E = F = 0$. In table 1 we give the actual values the canonical coefficients after the transformation corresponding to the results shown in figure 2.

Proof. For convenience, we consider the complexified phase space $z = x + iy$, so that the wavefunction (4) results in

$$\psi(z, \bar{z}, t) = (\hat{A} e^{-it} + \hat{B} e^{-2it} z + \hat{C} e^{-2it} \bar{z}) e^{-\frac{1}{2} z \bar{z}},$$

where $\sqrt{\pi} \hat{A} = A + iD$, $\sqrt{2\pi} \hat{B} = B + C + i(E - F)$ and $\sqrt{2\pi} \hat{C} = B - C + i(E + F)$. Then it is easy to check that the vortex, i.e. the set of points where the wavefunction vanishes, has the following position with respect to time:

$$z_v(t) = \frac{-|\hat{A}||\hat{B}| e^{i(t-b+a)} + |\hat{A}||\hat{C}| e^{-i(t-c+a)}}{|\hat{B}|^2 - |\hat{C}|^2},$$

where $\hat{A} = |\hat{A}| e^{ia}$, $\hat{B} = |\hat{B}| e^{ib}$ and $\hat{C} = |\hat{C}| e^{ic}$. Note that the vortex is well defined thanks to the non-degeneracy assumption, and its trajectory⁵ follows an ellipse. This ellipse does not appear in the usual canonical form, but this can be made so by performing the rotation: $z \mapsto z e^{i\mu}$ and the time shift: $t \mapsto t + \lambda$. In this way

$$z_v(t) = \frac{-|\hat{A}||\hat{B}| e^{i(t-b+a-\mu+\lambda)} + |\hat{A}||\hat{C}| e^{-i(t-c+a+\mu+\lambda)}}{|\hat{B}|^2 - |\hat{C}|^2},$$

where it is clear that by choosing $2\mu = c - b$ and $2\lambda = c + b - 2a$, the desired result is obtained. Then the corresponding wavefunction in these new coordinates is

$$\psi = (|\hat{A}| e^{-it} + |\hat{B}| e^{-2it} z + |\hat{C}| e^{-2it} \bar{z}) e^{-\frac{1}{2} z \bar{z}} e^{i(2a - \frac{b+c}{2})}$$

that can be further simplified since the factor $e^{i(2a - \frac{b+c}{2})}$ plays no role in the Bohmian equations for the quantum trajectories. Finally, by recovering the coefficients in cartesian coordinates, one obtains $\hat{A} = \sqrt{\pi} |\hat{A}|$, $\hat{B} = \sqrt{\frac{\pi}{2}} (|\hat{B}| + |\hat{C}|)$, $\hat{C} = \sqrt{\frac{\pi}{2}} (|\hat{B}| - |\hat{C}|)$ and $\hat{D} = \hat{E} = \hat{F} = 0$, which renders equation (7). $\square$

4. Study of the canonical form

Throughout the rest of the paper we consider the wavefunction (4) with $A, C \neq 0$, $B > 0$ and $D = E = F = 0$. Let us remark that by changing the time $t \mapsto -t$, if necessary, we can further restrict the study to the case $C > 0$. The corresponding quantum trajectories are then obtained from the vector field

$$X_\psi = \left(\frac{-2BCy - \sqrt{2}AB \sin t}{V(x, y, t)}, \frac{2BCx + \sqrt{2}AC \cos t}{V(x, y, t)} \right), \quad (8)$$

⁵ We use here the term trajectory to refer to the evolution of the vortex, despite the fact that it is not a solution of the ODE.

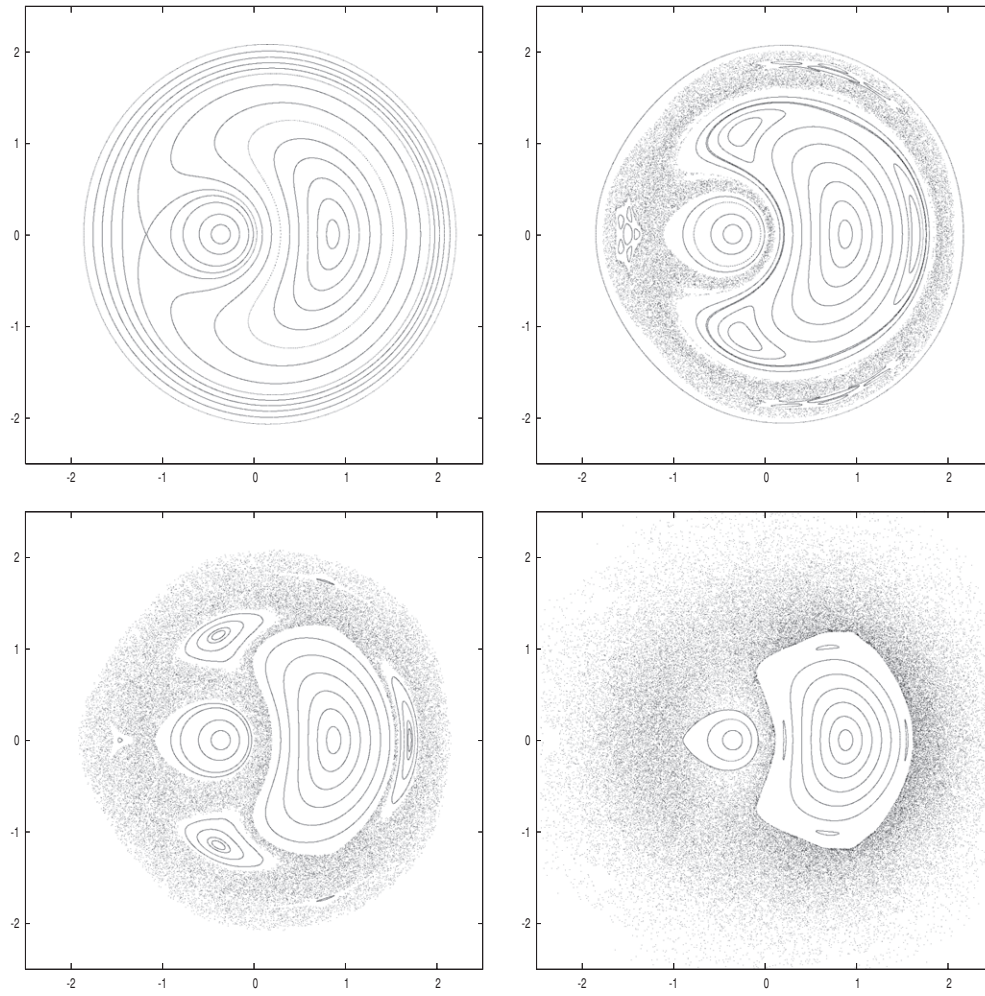


Figure 3. Stroboscopic 2π -periodic sections corresponding to the quantum trajectories generated by the canonical velocity field defined by equation (8) for $a = 0.4$, and $b = 0.4, 0.44, 0.48$ and 0.68 from left-top to right-bottom, respectively.

where $V(x, y, t) = 2B^2x^2 + 2C^2y^2 + 2\sqrt{2}ABx \cos t + 2\sqrt{2}ACy \sin t + A^2$. In these coordinates, the only vortex of the system follows the trajectory given by

$$(x_v(t), y_v(t)) = \left(-\frac{A}{\sqrt{2}B} \cos t, -\frac{A}{\sqrt{2}C} \sin t \right),$$

which corresponds to an ellipse of semi-axes $a = A/(\sqrt{2}B)$ and $b = A/(\sqrt{2}C)$, respectively.

In figure 3 we show some stroboscopic sections corresponding to this (canonical) velocity field for different values of the parameters a and b . As can be seen, a wide variety of dynamical behaviors, characteristics of a system with mixed dynamics, is found. In the left-top panel, which corresponds to the case in which $a = b$ (vortex moving in a circle), we have sections corresponding to a totally integrable case. As we move from left to right and top to bottom some of these tori are broken, and these areas of stochasticity coexist with others in which the

motion is regular, this including different chains of islands. Moreover, the size of the chaotic regions grows as the value of b separates from that of a .

This variety of results can be well understood and rationalized by using some standard techniques of the field of dynamical systems, in the following way. Although the vector field (8) is not Hamiltonian, it is time-reversible with respect to the involution $\Theta(x, y) = (x, -y)$. This result is very important for the purpose of the present paper, since it implies that the KAM theory applies to our system if we are able to write down our vector field in the form $X_\psi = X_0 + \varepsilon X_1$, $\varepsilon \ll 1$, being the dynamics corresponding to X_0 integrable and X_1 time-reversible. More specifically, let us assume that X_0 does not depend on t and X_1 be 2π -periodic with respect to t . Moreover, let us assume that for X_0 there exists a family of periodic orbits whose frequency varies along the family (non-degeneracy condition). Then our result guarantees that when the effect of the perturbation εX_1 is considered, most of the previous periodic orbits give rise to invariant tori of frequencies $(1, \omega)$, where ω is the frequency of the unperturbed periodic orbit. Of course, the persistence of these objects is conditioned to the fact that the vector $(1, \omega)$ satisfies certain arithmetic conditions (see [27, 28] for details). Since these arithmetic conditions are fulfilled for a big (in the sense of the Lebesgue measure) set of the initial orbits, the important hypothesis that we have to check in order to ascertain the applicability of the KAM theory is the non-degeneracy of the frequency map.

In our problem, two such integrable cases exist. First, if $A = 0$, the vortex is still at the origin and the time periodic part in the vector field disappears. As a consequence, all the quantum orbits of the system appear as ellipses centered at the origin in the xy -plane. It will be shown in the next section that the corresponding frequency varies monotonically along the orbits. This case has not been explicitly included in figure 3 due to its simplicity. Second, and as will be analyzed in section 6, if $B = C$, or equivalently $a = b$, that is the vortex moves in a circle, the vector field is also integrable for any value of A . The corresponding stroboscopic sections are shown in the top-left panel of figure 3). Here, the structure of the phase space changes notably, since two new periodic orbits, one stable and the other unstable, appear. Moreover, the obtained integrable vector field depends on t . We will show that this time dependence can be eliminated by means of a suitable change of coordinates, showing that our problem remains in the context described in the previous paragraph. The rest of the panels shown in figure 3 can be understood as the evolution of this structure as the perturbation, here represented by the difference between B and C , as dictated by the KAM theorem.

To conclude the paper, let us now discuss in detail the two integrable cases in the next two sections.

5. The integrable autonomous case

For $A = 0$, $B \neq 0$ and $C \neq 0$ it is easily seen that the vector field (8) is integrable. Actually, the orbits of the quantum trajectories in the xy -plane are ellipses around the origin (position at which the vortex is fixed). Also, the frequency of the corresponding trajectories approaches infinity as they get closer to the vortex position. Let us now compute the frequency ω of these solutions. First, we introduce a new time variable τ , satisfying $dt/d\tau = B^2x^2 + C^2y^2$, and then solve the resulting system, thus obtaining

$$x(\tau) = \alpha \cos(BC\tau + \beta), \quad y(\tau) = \alpha \sin(BC\tau + \beta), \quad (9)$$

where α is the distance from the vortex. Next, we recover the original time, t , by solving the differential equation defining the previous change of variables

$$\frac{dt}{d\tau} = \alpha^2 \frac{B^2 + C^2}{2} + \alpha^2 \frac{B^2 - C^2}{2} \cos(2BC\tau + 2\beta),$$

whose solution is given by

$$\underbrace{\frac{2}{\alpha^2(B^2 + C^2)}}_{\gamma} t = \tau + \underbrace{\frac{B^2 - C^2}{2(B^2 + C^2)BC}}_{\delta} \sin(2BC\tau + 2\beta).$$

Note that this equation is invertible since $|2BC\delta| < 1$, and then $\tau = \gamma t + f(2BC\gamma t)$, f being a 2π -periodic function. Finally, introducing this expression into (9), one can conclude that the solution has a frequency given by

$$\omega = BC\gamma = \frac{2BC}{\alpha^2(B^2 + C^2)}$$

that varies monotonically with respect to the distance to the vortex. Then, for $A \ll 1$, the existence of invariant tori around the vortex is guaranteed.

6. The integrable non-autonomous case

Let us consider now the case of non-vanishing values of $B = C$ for any $A \neq 0$. In this case, we have $a = b \neq 0$, and system (8) can be written as

$$X_\psi(x, y, t) = \left(\frac{-y - a \sin(t)}{\tilde{V}(x, y, t)}, \frac{x + a \cos(t)}{\tilde{V}(x, y, t)} \right), \quad (10)$$

where $\tilde{V}(x, y, t) = (x + a \cos(t))^2 + (y + a \sin(t))^2$. This vector field corresponds to the following Hamiltonian:

$$H(x, y, t) = -\frac{1}{2} \ln \tilde{V}(x, y, t)$$

that it is actually integrable.

Lemma 6.1. *Let us consider e (energy), the symplectic variable conjugate to t , and define the autonomous Hamiltonian $\mathcal{H}_1(x, y, t, e) = H(x, y, t) + e$; then we have that*

$$\mathcal{H}_2(x, y, t) = \tilde{V}(x, y, t) e^{-x^2 - y^2}$$

is a first integral of $\mathcal{H}_1$, in involution and functionally independent. As a consequence, if $a = b \neq 0$, the system is completely integrable.

Proof. It is straightforward to see that the Poisson bracket with respect to the canonical form $dx \wedge dy + dt \wedge de$ satisfies $\{\mathcal{H}_1, \mathcal{H}_2\} = 0$. Moreover, $\mathcal{H}_2$ does not depend on e , so that it is an independent first integral. $\square$

Taking these results into account, one can completely understand the picture presented in the top-left plot of figure 3. Since the system is integrable, it is foliated by invariant tori, despite the two periodic orbits that are created by a resonance introduced when parameter A changes from $A = 0$ to $A \neq 0$. Next, we characterize these two periodic orbits:

Lemma 6.2. *If $A > 0$, the system has two periodic orbits given by*

$$r_\pm(t) = (x_\pm(t), y_\pm(t)) = (a_\pm \cos t, a_\pm \sin t),$$

where the coefficients a_+ and a_- are given by $a_\pm = \frac{-a \pm \sqrt{a^2 + 4}}{2}$. Moreover, the orbit $r_-(t)$ is hyperbolic with characteristic exponents $\pm(a_-^4 - 1)^{1/2}$, and $r_+(t)$ is elliptic with characteristic exponents $\pm i(1 - a_+^4)^{1/2}$. If $A < 0$ the same result holds just switching the roles of a_+ and a_- .

Proof. It is known that if the sets $\{\mathcal{H}_2^{-1}(c), c \in \mathbb{R}\}$ are bounded differentiable submanifolds, their connected components carry quasi-periodic dynamics. Moreover, the critical points of

$\mathcal{H}_2$ determine the periodic orbits of the system. Therefore, these periodic orbits are given by expressions $2x\tilde{V} = \frac{\partial \tilde{V}}{\partial x}$, and $2y\tilde{V} = \frac{\partial \tilde{V}}{\partial y}$, which can also be written as

$$\begin{aligned} x((x+a\cos t)^2 + (y+a\sin t)^2) &= x+a\cos t, \\ y((x+a\cos t)^2 + (y+a\sin t)^2) &= y+a\sin t, \end{aligned}$$

from which we obtain our two periodic orbits: $x_{\pm}(t) = a_{\pm}\cos t$, and $y_{\pm}(t) = a_{\pm}\sin t$, with $a_{\pm} = 1/(a_{\pm} + a)$. In addition, it is easy to check that $a_{-}^2 > 1$ and $a_{+}^2 < 1$, respectively.

Finally, the stability of these orbits can be obtained by considering the following associated variational equations:

$$\begin{pmatrix} \dot{w}_1 \\ \dot{w}_2 \end{pmatrix} = a_{\pm}^2 \begin{pmatrix} \sin(2t) & -\cos(2t) \\ -\cos(2t) & -\sin(2t) \end{pmatrix} \begin{pmatrix} w_1 \\ w_2 \end{pmatrix}. \quad (11)$$

Solutions for this equation can be easily obtained by using the complex variable $z = w_1 + iw_2$, and solving $\dot{z} = -ie^{2it}a_{\pm}^2\bar{z}$. We have the following set of fundamental solutions:

$$\begin{aligned} w_1(t) &= e^{\pm it\sqrt{a_{\pm}^4-1}}((1-a_{\pm}^2)\cos t \mp \sqrt{a_{\pm}^4-1}\sin t), \\ w_2(t) &= e^{\pm it\sqrt{a_{\pm}^4-1}}((1-a_{\pm}^2)\sin t \pm \sqrt{a_{\pm}^4-1}\cos t), \end{aligned}$$

for the hyperbolic case, and

$$\begin{aligned} w_1(t) &= \cos(\pm t\sqrt{1-a_{+}^4})(\pm\sqrt{1-a_{+}^4}\cos t - (1+a_{+}^2)\sin t) \\ &\quad + \sin(\pm t\sqrt{1-a_{+}^4})(\pm\sqrt{1-a_{+}^4}\cos t + (1+a_{+}^2)\sin t), \\ w_2(t) &= \cos(\pm t\sqrt{1-a_{+}^4})(\pm\sqrt{1-a_{+}^4}\sin t + (1+a_{+}^2)\cos t) \\ &\quad + \sin(\pm t\sqrt{1-a_{+}^4})(\pm\sqrt{1-a_{+}^4}\sin t - (1+a_{+}^2)\cos t), \end{aligned}$$

for the elliptic one. Finally, the corresponding characteristic exponents can be obtained by a straightforward computation of the monodromy matrix. $\square$

Remark 6.3. Note that the chaotic sea observed in figure 3 is associated with the intersection of the invariant manifolds of the hyperbolic periodic orbit that we have computed.

Now, and in order to apply the KAM theorem, we compute locally the frequency map of this unperturbed system around the vortex and the elliptic periodic orbit. To this end, we perform a symplectic change of coordinates in a neighborhood of these objects in order to obtain action-angle variables up to third order in the action.

In general, let $\mathcal{H}(x, y, t, e) = H(x, y, t) + e$ be a Hamiltonian that is 2π -periodic with respect to t and has a first integral, $F(x, y, t)$. Let us consider the generating function, $\tilde{S}(x, t, I, E) = tE + S(x, t, I)$, determining a symplectic change of variables $(x, y, t, e) \mapsto (I, \theta, t, E)$ defined implicitly by

$$y = \frac{\partial S}{\partial x}, \quad e = E + \frac{\partial S}{\partial t}, \quad \theta = \frac{\partial S}{\partial I}$$

where θ is also 2π -periodic. This transformation is introduced in such a way that the new Hamiltonian depends only on I :

$$H\left(x, \frac{\partial S}{\partial x}, t\right) + \frac{\partial S}{\partial t} = h(I). \quad (12)$$

Since a first integral of the system is known, we can define the corresponding action as

$$I = F(x, y, t) = F\left(x, \frac{\partial S}{\partial x}, t\right). \quad (13)$$

From equation (13), we obtain locally the equation $\frac{\partial S}{\partial x} = f(x, t, I)$, so that we have $S(x, t, I) = \int f(x, t, I) dx + g(t, I)$. Introducing this expression into (12), we obtain the following equation for g :

$$\frac{\partial g}{\partial t} = h(I) - H(x, f, t) - \int \frac{\partial f}{\partial t} dx \quad (14)$$

and can conclude that since g must be 2π -periodic with respect to t , then $h(I)$ has to satisfy

$$h(I) = \left\langle H(x, f, t) + \int \frac{\partial f}{\partial t} dx \right\rangle = \langle H(x, f, t) \rangle, \quad (15)$$

where $\langle \cdot \rangle$ denotes average with respect to t . Finally, we note that since F is a first integral, we can define g so that θ becomes 2π -periodic.

Computations are simplified observing that the left-hand side of equation (14) does not depend on x (we use the fact that F is a first integral), so we can set $x = 0$. According to this, we have to solve $\hat{F}(\hat{f}, t) = I$, where $\hat{F}(\cdot, t) = F(0, \cdot, t)$ and then we have to compute the average $h(I) = \langle \hat{H}(\hat{f}, t) \rangle$, where $\hat{H}(\cdot, t) = H(0, \cdot, t)$.

First, let us consider a neighborhood of the vortex for $A > 0$. To this end, we introduce the new variables $x = -a \cos t + \Delta_x$ and $y = -a \sin t + \Delta_y$, so that the Hamiltonian $H_v = H_v(\Delta_x, \Delta_y, t)$ and the first integral $F_v = F_v(\Delta_x, \Delta_y, t)$ are

$$\begin{aligned} H_v &= -\frac{1}{2} \ln(\Delta_x^2 + \Delta_y^2) - a \Delta_x \cos t - a \Delta_y \sin t, \\ F_v &= (\Delta_x^2 + \Delta_y^2) \exp(-a^2 + 2a \Delta_x \cos t + 2a \Delta_y \sin t - \Delta_x^2 - \Delta_y^2). \end{aligned} \quad (16)$$

Proposition 6.4. *There exists a symplectic change of variables $(\Delta_x, \Delta_y, t, e) \mapsto (I, \theta, t, E)$, with $\theta \in \mathbb{T}$, setting the vortex at $I = 0$, such that the new Hamiltonian becomes*

$$h_v(I) = -\frac{1}{2} \ln I - \frac{a^2}{2} - \frac{e^{a^2} I}{2} - \frac{3a^2 e^{2a^2}}{2} I^2 + \mathcal{O}_3(I).$$

Proof. According to the above discussion, we have $\hat{F}_v(\hat{f}_v, t) = \hat{f}_v^2 e^{-a^2 + 2a \hat{f}_v \sin t - \hat{f}_v^2} = I$. Then by introducing this expression in (16) one obtains

$$\hat{H}_v(\hat{f}_v, t) = -\frac{1}{2} \ln I - \frac{a^2}{2} - \frac{\hat{f}_v^2}{2}.$$

Finally, we only have to compute the first terms in the expansion of $\hat{f}_v^2$ obtaining

$$\hat{f}_v^2 = e^{a^2} I - 2a e^{\frac{3}{2}a^2} \sin t I^{3/2} + 6a^2 e^{2a^2} \sin^2 t I^2 + \dots$$

and use that $\langle \sin t \rangle = 0$ and $\langle \sin^2 t \rangle = \frac{1}{2}$. $\square$

On the other hand, a neighborhood of the elliptic periodic orbit for $A > 0$ can be studied by means of the variables $x = a_+ \cos t + \Delta_x$ and $y = a_+ \sin t + \Delta_y$. One thus obtains that the Hamiltonian and the first integral are given by

$$\begin{aligned} H_+ &= -\frac{1}{2} \ln V_+ + a_+ \Delta_x \cos t + a_+ \Delta_y \sin t, \\ F_+ &= V_+ \exp(-a_+^2 - 2a_+ \Delta_x \cos t - 2a_+ \Delta_y \sin t - \Delta_x^2 - \Delta_y^2), \end{aligned}$$

where $V_+ = (a + a_+)^2 (1 + 2a_+ \Delta_x \cos t + 2a_+ \Delta_y \sin t + a_+^2 \Delta_x^2 + a_+^2 \Delta_y^2)$.

Proposition 6.5. *There exists a symplectic change of variables $(\Delta_x, \Delta_y, t, e) \mapsto (I, \theta, t, E)$, with $\theta \in \mathbb{T}$, setting the periodic orbit at $I = (a_+ + a)^2 e^{-a^2}$, such that the new Hamiltonian becomes*

$$h_+(I) = -\ln(a + a_+)^2 + \frac{1 - \Pi_1}{2} J - \frac{1 + 2\Pi_2}{4} J^2 + \mathcal{O}_3(I),$$

where we have introduced the notation

$$J = 1 - \frac{e^{a^2} I}{(a_+ + a)^2}$$

and also

$$\Pi_1 = \frac{1}{\sqrt{1 - a_+^4}}, \quad \Pi_2 = \frac{a^2(41a^8 - 88a^6 + 119a^4 - 54a^2 + 18)}{36\sqrt{1 - a_+^4}(a^8 + 1 - 2a^4)(1 + a^2)}.$$

Proof. As before, we consider a solution $\hat{f}_+(I, t)$ for the equation $\hat{F}_+(\hat{f}_+, t) = I$. For convenience, we introduce the notation $I = (a_+ + a)^2 e^{-a^2} (1 - J)$ in order to set the periodic orbit at $J = 0$. Then it turns out that the expression

$$(1 - a_+^2 \cos(2t)) \hat{f}_+^2 + (a_+(1 + a^2) \sin t - \frac{8}{3} a_+^3 \sin^3 t) \hat{f}_+^3 + \mathcal{O}_4(\hat{f}_+) = J$$

approximates the previous equation for $\hat{f}_+$ and that the following expansion in terms of J

$$\hat{f}_+^2 = \alpha_1(t) J + \alpha_{3/2}(t) J^{3/2} + \alpha_2(t) J^2 + \dots$$

holds, where

$$\begin{aligned} \alpha_1(t) &= \frac{1}{1 - a_+^2 \cos 2t}, \\ \alpha_{3/2}(t) &= \frac{-a_+(1 + a_+^2) \sin t + \frac{8}{3} a_+^3 \sin^3 t}{(1 - a_+^2 \cos(2t))^{5/2}}, \\ \alpha_2(t) &= \frac{3}{2} \frac{(a_+(1 + a_+)^2 \sin t - \frac{8}{3} a_+^3 \sin^3 t)^2}{(1 - a_+^2 \cos 2t)^4}. \end{aligned}$$

Hence, we have to compute the average of

$$\hat{H}_+(\hat{f}_+, t) = -\ln(a_+ + a)^2 - \frac{1}{2} \ln(1 - J) - \frac{\hat{f}_+^2}{2}$$

that follows from the fact that $\langle \alpha_1 \rangle = \Pi_1$, $\langle \alpha_{3/2} \rangle = 0$ and $\langle \alpha_2 \rangle = \Pi_2$. These averages are computed easily by using the method of residues. $\square$

7. Conclusion

In this paper we present a scheme to study in a systematic way the intrinsic stochasticity and general complexity of the quantum trajectories that are the basis of quantum mechanics in the formalism developed by Bohm in the 1950s. In our opinion this approach, which is based on the ideas and results of the dynamical systems theory, can seriously contribute to establish firm grounds that foster the importance of the conclusions of future studies relying on such trajectories, thus avoiding errors and ambiguities that happened in the past. As an illustration we have considered the simplest, non-trivial combination of eigenstates of the two-dimensional isotropic harmonic oscillator.

The corresponding velocity field is put in a so-called canonical form, and the characteristics of the corresponding quantum trajectories studied in detail. It is proved that

Table 2. Dynamical characteristics of the quantum trajectories generated from the different possibilities in the canonical model (8) for the pilot wavefunction (4).

	Integrable	Hamiltonian	Time-reversible	Stroboscopic sections
$A = 0, B \neq 0, C \neq 0$	Yes	No	Yes	Ellipses around origin
$A \neq 0, B = C$	Yes	Yes	Yes	Top-left panel in figure 3
$A \neq 0, B \neq C$	No	No	Yes	Rest of panels in figure 3

only one vortex and two periodic orbits, one elliptic and the other hyperbolic, organize the full dynamics of the system. In it, there exist invariant tori associated with the vortex and the elliptic periodic orbit. Moreover, there is a chaotic sea associated with the hyperbolic periodic orbit. The KAM theory has been applied to this scenario by resorting to a suitable time-reversible symmetry, that is directly observed in the canonical form for the velocity field determining the quantum trajectories of the system. It should be remarked that the results reported here concerning the hyperbolic periodic orbit constitute a generalization of those previously reported in [15], in the sense that here a more concise and constructive approach to the associated dynamics is presented. We summarize the dynamical characteristics of the different possibilities arising from the canonical velocity field (8) in table 2, that represents a true road-map to navigate across the dynamical system, i.e. quantum trajectories, that are defined based on the pilot effect [3] of the wavefunction (4). Also, note that the generic model, i.e. when E , F or G do not vanish, does not satisfy any of the properties considered in the table.

Finally, the method presented here is, in principle, generalizable to other more complicated situations in which more vortex and effective dimensions exist. Some methods have been described in the literature that can be applied to these situations [30]. This will be the subject of future work.

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References

- [1] Feynman R P and Hibbs A R 1965 *Quantum Mechanics and Path Integrals* (New York: McGraw-Hill)
- [2] von Neumann J 1955 *Mathematical Foundations of Quantum Mechanics* (Princeton, NJ: Princeton University Press)
- [3] Bohm D 1952 *Phys. Rev.* **85** 166
- [4] Holland P 1995 *The Quantum Theory of Motion* (Cambridge: Cambridge University Press)
- [5] Wyatt R E 2005 *Quantum Dynamics with Trajectories. Introduction to Quantum Hydrodynamics* (New York: Springer)
- [6] Makri N 2004 *J. Phys. Chem. A* **108** 806
- [7] Liu J and Makri N 2004 *J. Phys. Chem. A* **108** 5408
- [8] Lopreore C L and Wyatt R E 1999 *Phys. Rev. Lett.* **82** 5190
- [9] González J, González M F, Bofill J M and Giménez X 2005 *J. Mol. Struct. THEOCHEM* **727** 205
- [10] Gindensperger E, Meyer C and Beswick J A 2002 *J. Chem. Phys.* **116** 8

- [11] Sanz A S, Borondo F and Miret-Artes S 2004 *Phys. Rev. B* **69** 115413
- [12] Prezhdo O V and Brooksby C 2001 *Phys. Rev. Lett.* **86** 3215
- [13] Sanz A S, Borondo F and Miret-Artes S 2001 *Europhys. Lett.* **55** 303
- [14] Frisk H 1997 *Phys. Lett. A* **227** 139
- [15] Wisniacki D A and Pujals E R 2005 *Europhys. Lett.* **71** 159
- [16] Wisniacki D A, Pujals E R and Borondo F 2006 *Europhys. Lett.* **73** 671
- [17] Wisniacki D A, Pujals E R and Borondo F 2007 *J. Phys. A: Math. Theor.* **40** 14353
- [18] Efthymiopoulos C and Contopoulos G 2006 *J. Phys. A: Math. Gen.* **39** 1819
- [19] Durr D, Goldstein S, Tumulka R and Zanghi N 2004 *Phys. Rev. Lett.* **93** 4546
- [20] Valentini A and Westman H 2005 *Proc. R. Soc. A* **461** 253
- [21] Polavieja G G 1997 *Phys. Rev. A* **53** 2059
- [22] de Alcantara Bonfim O F, Florencio J and Barreto F C S 1999 *Phys. Rev. E* **58** 2693
- [23] Goldstein S 1999 *Phys. Rev. E* **60** 7578
- [24] Lichtenberg A J and Lieberman M A 1983 *Regular and Chaotic Dynamics* (New York: Springer)
- [25] Berry M 2000 *Nature* **403** 6765
- [26] Arnol'd V I 1984 *Nonlinear and Turbulent Processes in Physics* vol 3 (Chur: Hardwood Academic) pp 1161–74
- [27] Broer H W, Huitema G B and Sevryuk M B 1996 *Quasi-periodic Motions in Families of Dynamical Systems. Order Amidst Chaos* (Berlin: Springer)
- [28] Sevryuk M B 2007 *Discrete Contin. Dyn. Syst. Ser. A* **18** 569
- [29] Lázaro J T 2003 On normal forms and splitting of separatrices in reversible systems *PhD Thesis* at Universitat Politécnica de Catalunya
- [30] Broer H, Hanssmann H, Jorba Á, Villanueva J and Wagnen F 2003 *Nonlinearity* **16** 1751