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Quantum–classical correspondence of a field induced KAM-type transition: A QTM approach

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Abstract. A transition from regular to chaotic behaviour in the dynamics of a classical Henon–Heiles oscillator in the presence of an external field is shown to have a similar quantum signature when studied using the pertaining phase portraits and the associated Kolmogorov–Sinai–Lyapunov entropies obtained through the corresponding Bohmian trajectories.

Keywords. Quantum potential; Bohmian trajectories; Henon–Heiles oscillator; KAM transition.

1. Introduction

Many classical non-linear dynamical systems exhibit Kolmogorov–Arnold–Moser (KAM) transition[1–5] wherein the dynamics of the system changes from a regular to a chaotic one by varying the non-integrability parameter present in the Hamiltonian. A quantum variant of the KAM transition is the subject matter of current research interest.[6–17] Classical and quantum Henon–Heiles oscillators have been extensively studied for this purpose.[5,18] Various diagnostics like the initially close Bohmian trajectories and the associated Kolmogorov–Sinai–Lyapunov (KSL) entropies, phase portraits and phase space volume (uncertainty product), autocorrelation function and the related power spectrum, etc. have been used[18] in analysing the quantum domain behaviour of the classically chaotic Henon–Heiles oscillator as the degree of the non-linearity and non-integrability is increased.

In the present work, we start with the classical Henon–Heiles oscillator at the regular domain and expose it to an external field. As the intensity of the external field is increased it is expected that the oscillator dynamics will move from regular to chaotic as was noticed by Lin and Balentine[19] in the field induced barrier penetration in a double-well oscillator as well as in its quantum analogue.[20]

Quantum potential based approaches like quantum fluid dynamics (QFD)[21] and quantum theory of motion (QTM)[22] have been used in the past for understanding the quantum domain behaviour of these systems.[18,20,22–24] We make use of quantum potential based approaches in the present work to analyse the quantum analogue of the field induced KAM transition in a Henon–Heiles oscillator.

Sections 2 and 3 provide the theoretical background and the numerical technique adopted here. Results and discussion are presented in §4 while §5 contains some concluding remarks.

2. Theoretical background

The classical dynamics of the Henon–Heiles oscillator in presence of an axial external field applied in the y-direction is studied by solving the pertinent classical Hamilton's equations of motion with the following Hamiltonian:

$$H(x,y)=\frac{1}{2}(p_x^2+p_y^2)+\frac{1}{2}(x^2+y^2)$$
$$+\lambda x\left(y^2-\frac{x^2}{3}\right)-gy\cos(\omega t) \qquad (1)$$

where the first term stands for the kinetic energy, the second and the third terms respectively represent the harmonic and anharmonic parts of the potential energy of the oscillator whereas the last term takes care of the interaction of the oscillator with the external axial field. The non-linearity and the non-integrability parameter λ has a value of 0·1118034[5,8] and the system quantization is performed with $\hbar = 1$, $m = 1$.

The associated time-dependent Schrödinger equation (TDSE) is given by

*For correspondence

$$\left[-\frac{1}{2}\left(\frac{\partial^2}{\partial x^2}+\frac{\partial^2}{\partial y^2}\right)+\frac{1}{2}(x^2+y^2)\right.$$

$$\left.+\lambda x\left(y^2-\frac{x^2}{3}\right)-gy\cos(\omega t)\right]\psi(x,y,t)$$

$$=i\frac{\partial\psi(x,y,t)}{\partial t};\ i=\sqrt{-1} \tag{2}$$

The wavefunction $\psi(x, y, t)$ may be written in the following polar form in terms of the density, $\rho(x, y, t)$ and the velocity potential, $\chi(x, y, t)$:

$$\psi(x,y,t)=\rho^{1/2}(x,y,t)\exp[i\chi(x,y,t)], \tag{3}$$

and the velocity components may be defined as

$$\dot{x}=\nabla_x\chi(x,y,t)|_{x=x(t)}, \tag{4a}$$

and

$$\dot{y}=\nabla_y\chi(x,y,t)|_{y=y(t)} \tag{4b}$$

According to the quantum theory of motion (QTM),[22] the quantum (Bohm) trajectories may be generated by solving (4) with different initial conditions. A phase space distance function has been defined as,[18,20,23]

$$D(t)=\{[x_1(t)-x_2(t)]^2+[y_1(t)-y_2(t)]^2$$

$$+[p_{x_1}(t)-p_{x_2}(t)]^2+[p_{y_1}(t)-p_{y_2}(t)]^2\}^{1/2}, \tag{5}$$

where (x, p_x, y, p_y) denotes a representative phase point.

In analogy with the corresponding classical nonlinear dynamics study a generalized quantum Lyapunov exponent has also been defined[18,20,23] as,

$$\Lambda=\lim_{\substack{D(0)\to 0\\ t\to\infty}}\frac{1}{t}\ln\left[\frac{D(t)}{D(0)}\right] \tag{6}$$

and the corresponding Kolmogorov–Sinai–Lyapunov (KSL) entropy (H^{Qu}) has been given by,[18,20,23]

$$H^{Qu}=\sum_{\Lambda_+\succ 0}\Lambda_+ \tag{7}$$

3. Numerical technique

Classical Hamilton's equations of motion are solved using a fourth-order Runge–Kutta method. Once the phase points, (x, p_x, y, p_y) are known at different time steps the phase space trajectories and the classical KSL entropy (H^{Cl}) are generated.

For the quantum problem the TDSE is solved by using a Peaceman–Rachford type finite difference algorithm [25] using the following initial and boundary conditions:

$$\psi(x,y,t=0\ )=\frac{1}{\sqrt{\pi}}\exp\{-\tfrac{1}{2}[(x-x_o)^2+(y-y_o)^2]\} \tag{8a}$$

$$\psi(\pm\infty,y,t)=0\ \ \forall\ y,t \tag{8b}$$

$$\psi(x,\pm\infty,t)=0\ \ \ \forall\ x,t \tag{8c}$$

The Guassian wavepacket is propagated for several time steps and for $-10\le x, y\le 10$. Since the classical chaoticity requires more time to develop the classical solution is continued up to $2{\cdot}56\times10^3$ time steps. All the quantities are in atomic units unless otherwise specified. The mesh sizes adopted are $\Delta x=\Delta y=0{\cdot}08$. The temporal mesh sizes for the classical and quantum calculations are taken as $\Delta t=0{\cdot}128$ and $\Delta t=0{\cdot}0128$ respectively.

After obtaining $\psi(x, y, t)$ by solving the TDSE, (4) are solved using a second-order Runge–Kutta method to generate the Bohmian trajectories which allow us to obtain the quantum KSL entropies (H^{Qu}) by using (6) and (7). The initial separation of the trajectories is taken to be 10^{-5}.

4. Results and discussion

The left and the right panels of the figure 1 respectively present the classical and quantal phase-portraits (y, p_y) for four different field intensities. At $g=0$, a distinct torus is visible for the classical case. A cantorus like structure is obtained as the corresponding quantum analogue. As the field intensity increases the area of the phase space traversed by the trajectories increases and the system started exhibiting the typical Kolmogorov–Arnold–Moser type transition to the chaotic domain. In the quantum case also the corresponding transition is faithfully mimicked. In figure 1 we also present the classical and quantal phase space distance functions. For $g=0{\cdot}0$, $0{\cdot}1$ and $0{\cdot}5$ the initial small distance (10^{-5}) of two nearby

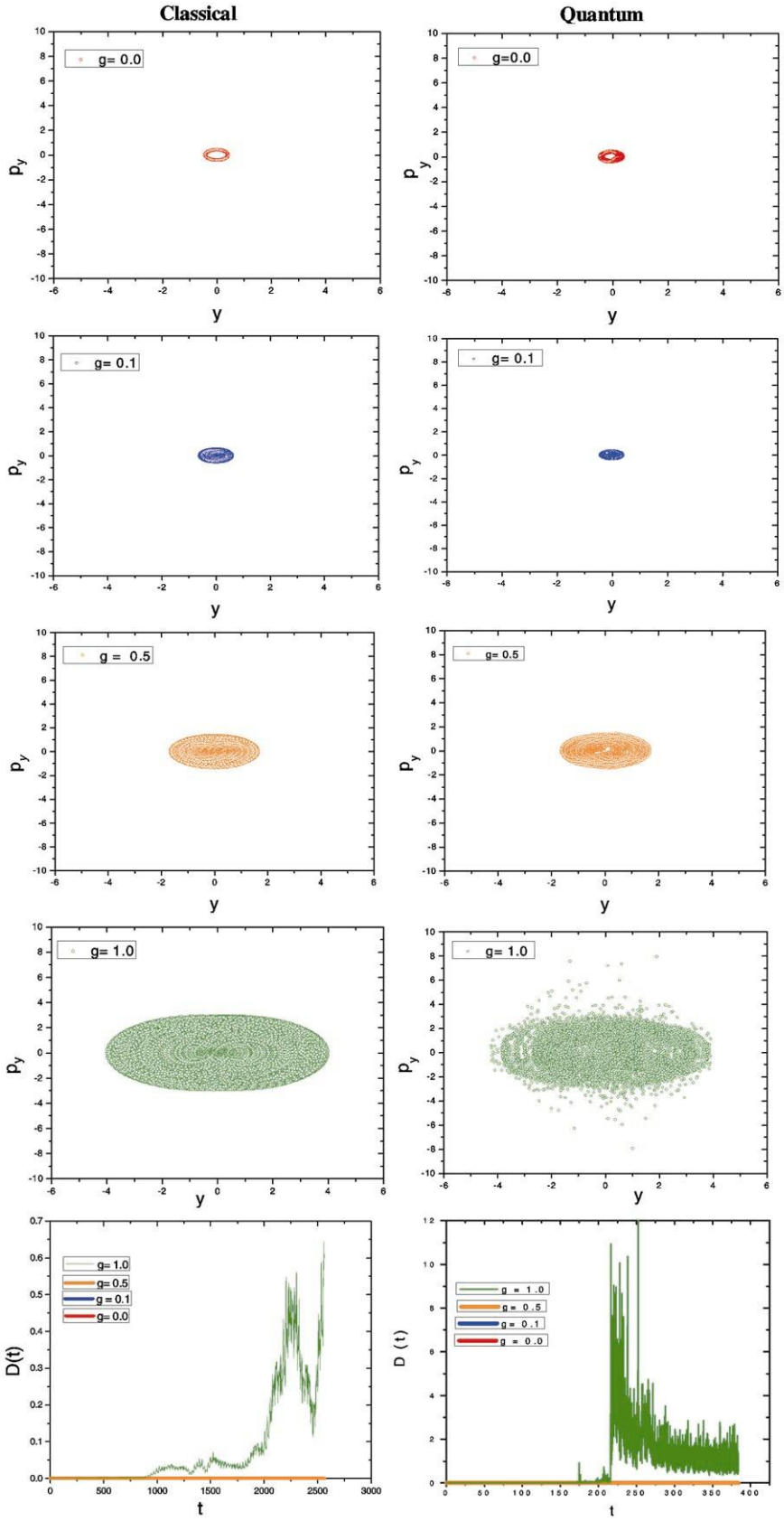

Figure 1. Classical and quantal phase portraits (p_y vs y) for the Henon–Heiles oscillator in the presence of an external field of varying intensities with g = 0·0, 0·1, 0·5 and 1·0. Also shown are the respective phase space distance functions ($D(t)$).

quantum trajectories is more or less maintained which, however, drastically increases for higher field intensity ($g = 1{\cdot}0$). Once again the quantum stochasticity is manifested much earlier. The oscillation in $D(t)$ might have a bearing in the associated wavefunction revival. It deserves a careful scrutiny.

Time evolution of the classical KSL entropy (H^{Cl}) is depicted in the figure 2. As the system perturbation, originating from the external field, is increased

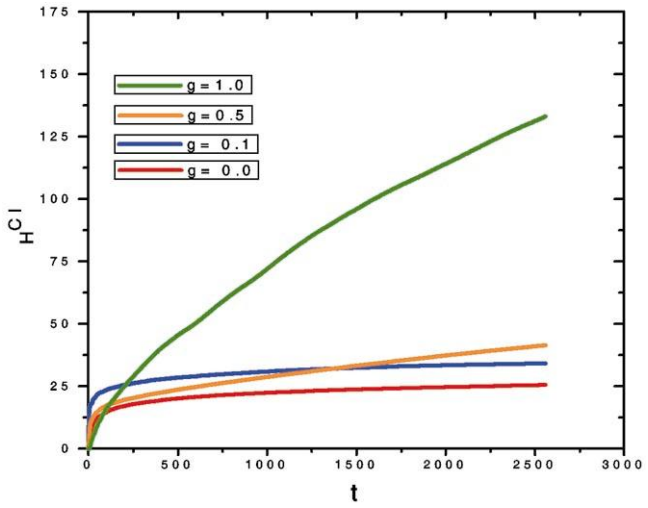

Figure 2. Time evolution of the KSL entropy associated with the classical motion (H^{Cl}) of the Henon–Heiles oscillator in the presence of an external field of varying intensities with $g = 0{\cdot}0$, $0{\cdot}1$, $0{\cdot}5$ and $1{\cdot}0$.

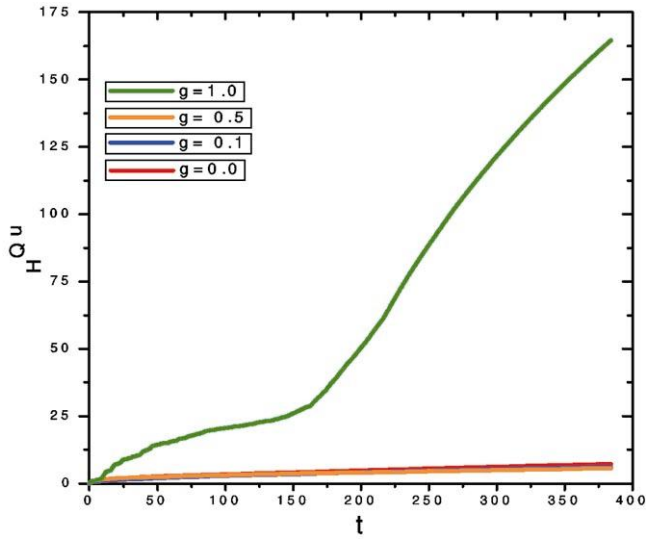

Figure 3. Time evolution of the KSL entropy associated with the quantal motion (H^{Qu}) of the Henon–Heiles oscillator in the presence of an external field of varying intensities with $g = 0{\cdot}0$, $0{\cdot}1$, $0{\cdot}5$ and $1{\cdot}0$.

there results a discernible jump in the entropy value, a clear-cut signature of classical chaos through KAM transition.

Figure 3 presents the variation of the quantum KSL entropy (H^{Qu}) as a function of time, for four different values of the external field intensity. It is interesting to note that there exists a one-to-one correspondence between the classical and quantum behaviour of the non-linear oscillator. The quantum signature of the classical chaos is conspicuous. Although the classical stochasticity enhances the quantum fluctuations ($g = 1{\cdot}0$), quantum non-classical effects somewhat suppress the classical chaos ($g = 0{\cdot}0$, $0{\cdot}1$, $0{\cdot}5$) as was observed[18,20,23] in various non-linear dynamical systems.

5. Concluding remarks

Quantum signature of the Kolmogorov–Arnold–Moser transition of a Henon–Heiles oscillator in the presence of the external field of varying intensities is studied using the quantum theory of motion. A clear-cut correspondence between the classical chaos and its quantum variant is observed in terms of the respective phase-portraits and the associated Kolmogorov–Sinai–Lyapunov entropies.

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