

Quantum signature of the classical chaos in the field-induced barrier crossing in a quartic potential*

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The quantum domain behaviour of a classical double-well oscillator which exhibits chaos in the presence of an external monochromatic field has been studied using Bohmian mechanics. The classical Kolmogorov–Arnol’d–Moser (KAM) tori break down in the presence of an external perturbation for which the corresponding quantal phase portrait exhibits regular islands owing to the quantum suppression of the classical chaos. It has also been observed that the classical chaos generally enhances the quantum fluctuations.

THERE has been a recent upsurge of interest in the study of the quantum dynamics of classically chaotic systems^{1–14}. It has been shown^{1–14} that the quantum nonclassical effects suppress the classical stochasticity. An integrable classical system or a system in the presence of a weak perturbation is characterized by invariant KAM tori. The phase space begins to appear chaotic when the amplitude of the external destabilizing field is increased¹⁵. The KAM tori in this case break down into cantori¹⁶ which help in stabilizing the corresponding quantum system^{13,14}. In order to understand these aspects better we study the quantum domain behaviour of a quartic oscillator in the presence of an external monochromatic field. This problem is considered to be important in several areas of chemical dynamics¹⁷ and has been studied in detail^{13–15} in recent years. It has been observed^{13,14} that the classical chaos and quantum tunneling occur simultaneously in this case to give rise to the coherent oscillatory nature of the quantum diffusion between two stable KAM tori.

Quantum potential based approaches^{1,18–20} offer a good quantum description of classically chaotic systems. In quantum fluid dynamics (QFD)¹⁸, the overall motion of the system is mapped onto the motion of a ‘probability fluid’ having density $\rho(\mathbf{r}, t)$ and velocity $v(\mathbf{r}, t)$ under the influence of the external classical potential augmented by a quantum potential. The basic equations of QFD comprise an equation of continuity and an Euler-type equation of motion. It has been shown⁹ that these equations can be written in the form of

Hamilton’s equations of motion with a Hamiltonian functional properly defined for this purpose and by considering $\rho(\mathbf{r}, t)$ and $(-\chi(\mathbf{r}, t))$ as canonically conjugate variables, where $\chi(\mathbf{r}, t)$ is the velocity potential. Chaotic dynamics of a quantum Hénon-Heiles oscillator has been studied⁹ using QFD, in terms of ρ versus $(-\chi)$ plots and time evolution of several time-dependent density functionals like Shannon entropy, density correlation and macroscopic kinetic energy. Another quantum potential-based theory is the quantum theory of motion (QTM)¹ in the sense of classical interpretation of quantum mechanics as developed by de Broglie¹⁹ and Bohm²⁰. In QTM¹, the overall motion of a physical system is understood in terms of both wave and particle pictures. The pertinent time-dependent Schrödinger equation (TDSE) governs the wave motion. This wave guides a point particle whose motion is described in terms of forces originating from the classical as well as quantum potentials. In QTM, important insights into quantum domain chaotic dynamics are obtained^{10,11} in terms of the phase space distance between two initially close Bohmian trajectories and the associated Kolmogorov–Sinai (KS) entropy. Quantum standard map¹¹, Weigert’s quantum cat map¹¹, Rydberg atoms in external fields¹⁰ and a quantum Hénon-Heiles oscillator¹⁰ have been studied successfully using QTM. Possibility of a QTM for many-electron systems is being explored²¹ within a quantum fluid density functional framework²².

In the present work, we apply QTM in analysing the quantum analogue of the classical domain chaotic dynamics associated with the penetration of a barrier in a double-well potential in the presence of a monochromatic external field with increasing amplitude.

The classical Hamiltonian of a double-well oscillator under the influence of an external oscillating driving force is given by:

$$\mathcal{H} = \frac{p^2}{2m} + ax^4 - bx^2 + c \cos(\omega_0 t). \quad (1)$$

For a given set of parameter values, the classical Hamilton’s equations of motion can be solved^{13,14} to generate the stroboscopic plots of various trajectories. Depending on the choice of the initial position and momentum values one may obtain stable regions in phase space bounded by KAM surfaces or a chaotic sea extended over the whole phase space.

In order to get a quantum mechanical description of this problem, the classical Hamiltonian (eq. (1)) is directly quantized and the pertinent TDSE has been written as:

$$\begin{aligned} \hat{H}\psi(x, t) &= \left[-\frac{1}{2} \frac{d^2}{dx^2} + ax^4 - bx^2 + c \cos(\omega_0 t) \right] \psi(x, t) \\ &= i \frac{\partial \psi(x, t)}{\partial t}. \end{aligned} \quad (2)$$

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Atomic units are used throughout unless otherwise specified. The complete description of a physical system involves both wave and particle pictures in QTM¹. While the wave motion is governed by the TDSE, the motion of a point particle guided by this wave is characterized by its velocity as given by:

$$\dot{x} = \nabla\chi(x, t)|_{x=x(t)}, \quad (3)$$

where χ is the velocity potential expressed as the phase of the wavefunction in its polar form as follows:

$$\psi(x, t) = \rho^{1/2}(x, t) \exp[i\chi(x, t)]. \quad (4)$$

An assembly of initial positions will constitute an ensemble of particle motions guided by the same wave, and the probability that the particle be present between x and $x + dx$ in this ensemble at time t is given by $\rho(x, t)dx$. Solution of eq. (3) with various initial positions would yield the so-called 'Bohmian trajectories'. A phase space distance function can be defined as follows^{10,11} in order to study the quantum signature of chaos through sensitive dependence on initial conditions,

$$D(t) = \{(x_1(t) - x_2(t))^2 + (p_{x_1}(t) - p_{x_2}(t))^2\}^{1/2}, \quad (5)$$

where (x, p_x) refers to a point in phase space.

A generalized quantum Lyapunov exponent has also been defined as¹¹:

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

The corresponding KS entropy is given by¹¹:

$$H = \sum_{\Lambda_+ > 0} \Lambda_+. \quad (7)$$

Chaotic quantum dynamics is characterized by a positive KS entropy¹¹.

The phase space volume is defined as¹²:

$$V_{ps}(t) = [\langle (x - \langle x \rangle)^2 \rangle \langle (p_x - \langle p_x \rangle)^2 \rangle]^{1/2}. \quad (8)$$

A sharp increase in $V_{ps}(t)$ implies a chaotic motion^{10,12}. This quantity is same as the associated uncertainty product which can be used as a measure of quantum fluctuations¹⁴. Classical chaos generally enhances quantum fluctuations^{10,12,14}.

The double-well potential used in the present problem is given by:

$$V(x) = ax^4 - bx^2 + c \cos(\omega_0 t), \quad (9)$$

where the parameter values are taken as follows¹³: $a = 0.5$, $b = 10.0$, $c = 10.0$ and $\omega_0 = 6.07$. Classical phase-portraits and their QTM counterparts are generated for two different initial conditions, $(x, p_x)|_{t=0}$, viz. (a) $(-2.0, 0.0)$ and (b) $(2.0, 0.0)$. For the given set of parameter values the classical motion is regular for case (a) and chaotic for case (b) although both the cases correspond to the same value of the unperturbed energies of the double-well oscillator.

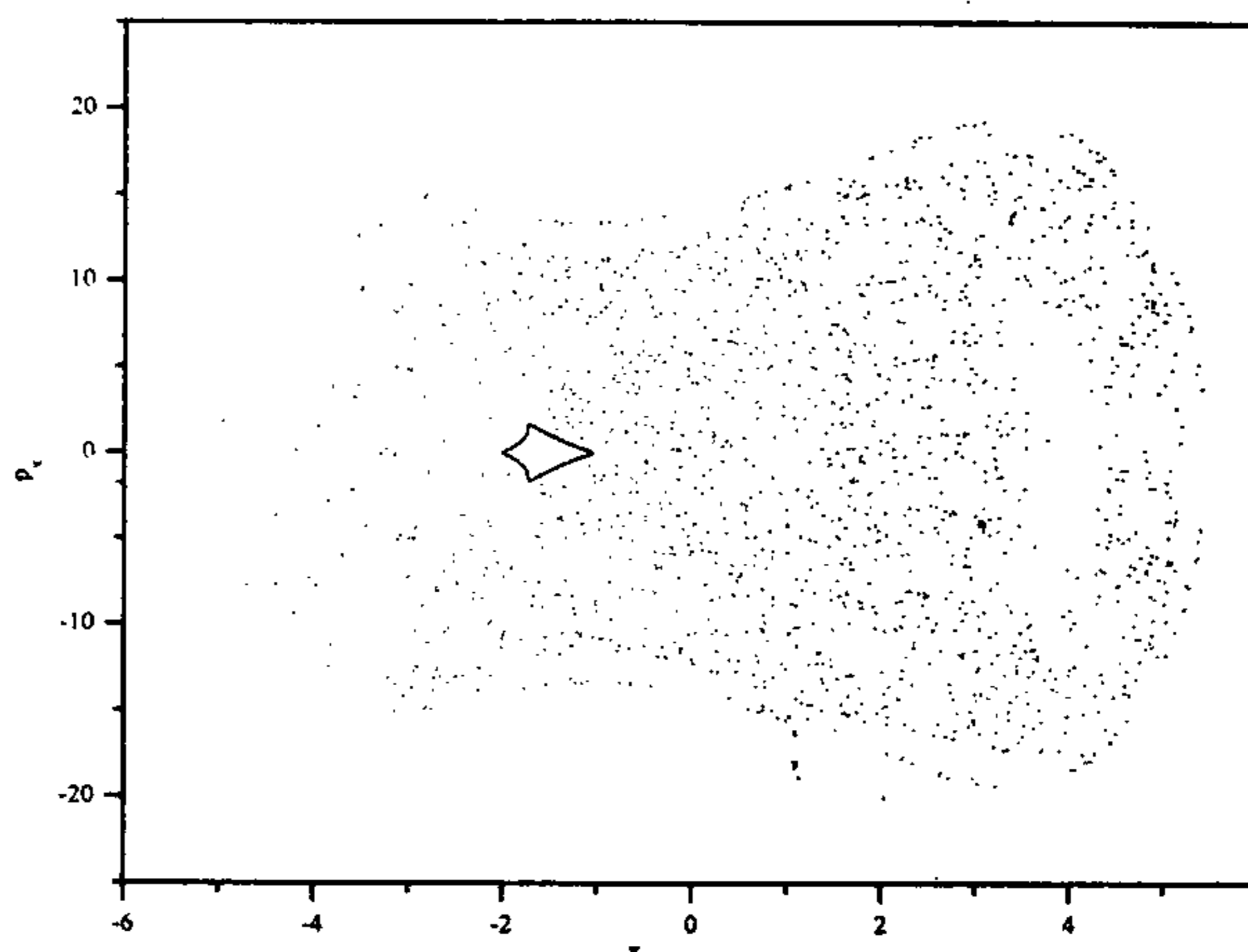


Figure 1. Classical phase space trajectories for a double-well oscillator in the presence of an external field with $c = 10$ and two different initial conditions: (a) $(x_0 = -2.0, p_0 = 0.0)$; (b) $(x_0 = 2.0, p_0 = 0.0)$.

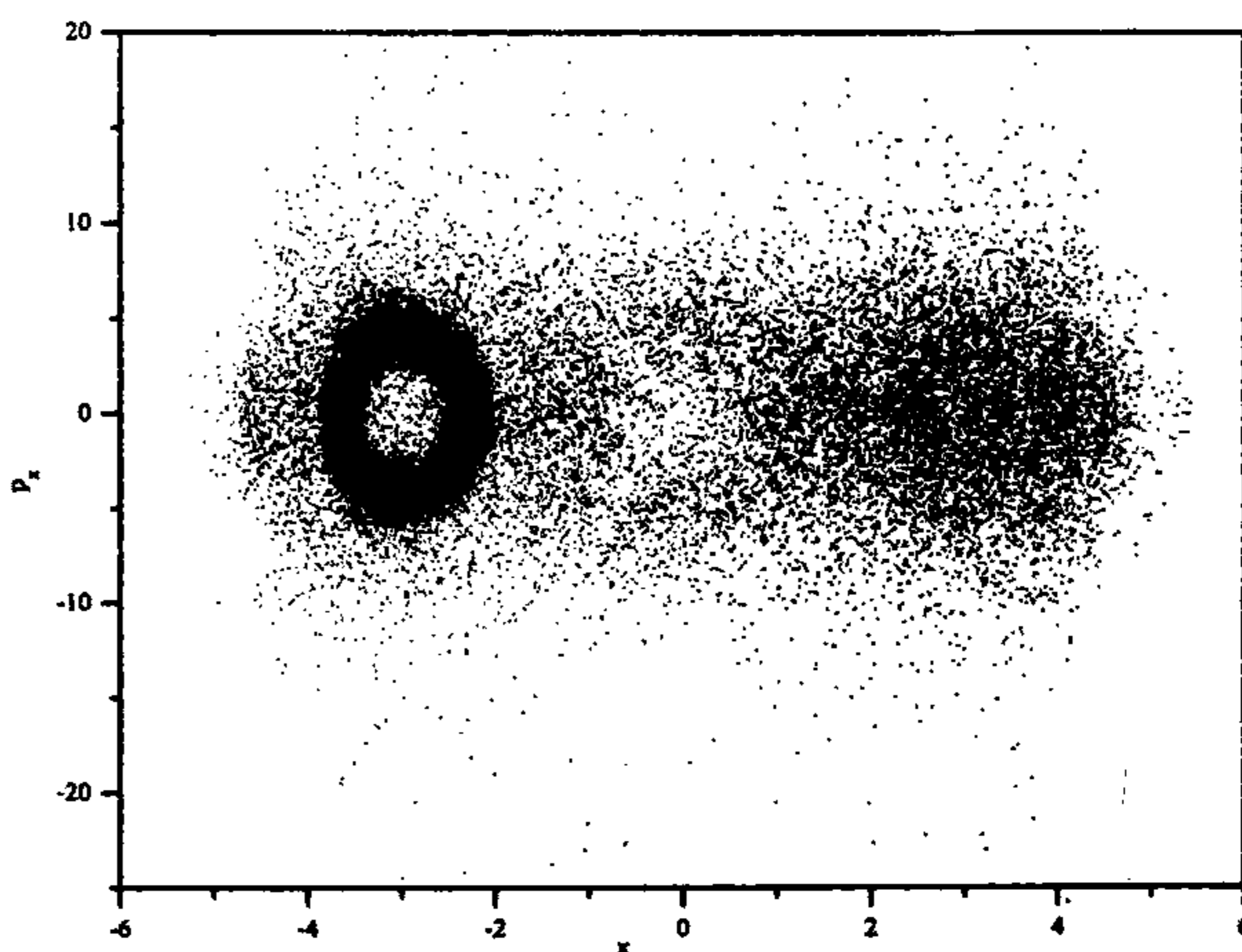


Figure 2. Quantal phase space trajectories for a double-well oscillator in the presence of an external field with $c = 10$ and two different initial conditions: (a) $(x_0 = -2.0, p_0 = 0.0)$; (b) $(x_0 = 2.0, p_0 = 0.0)$.

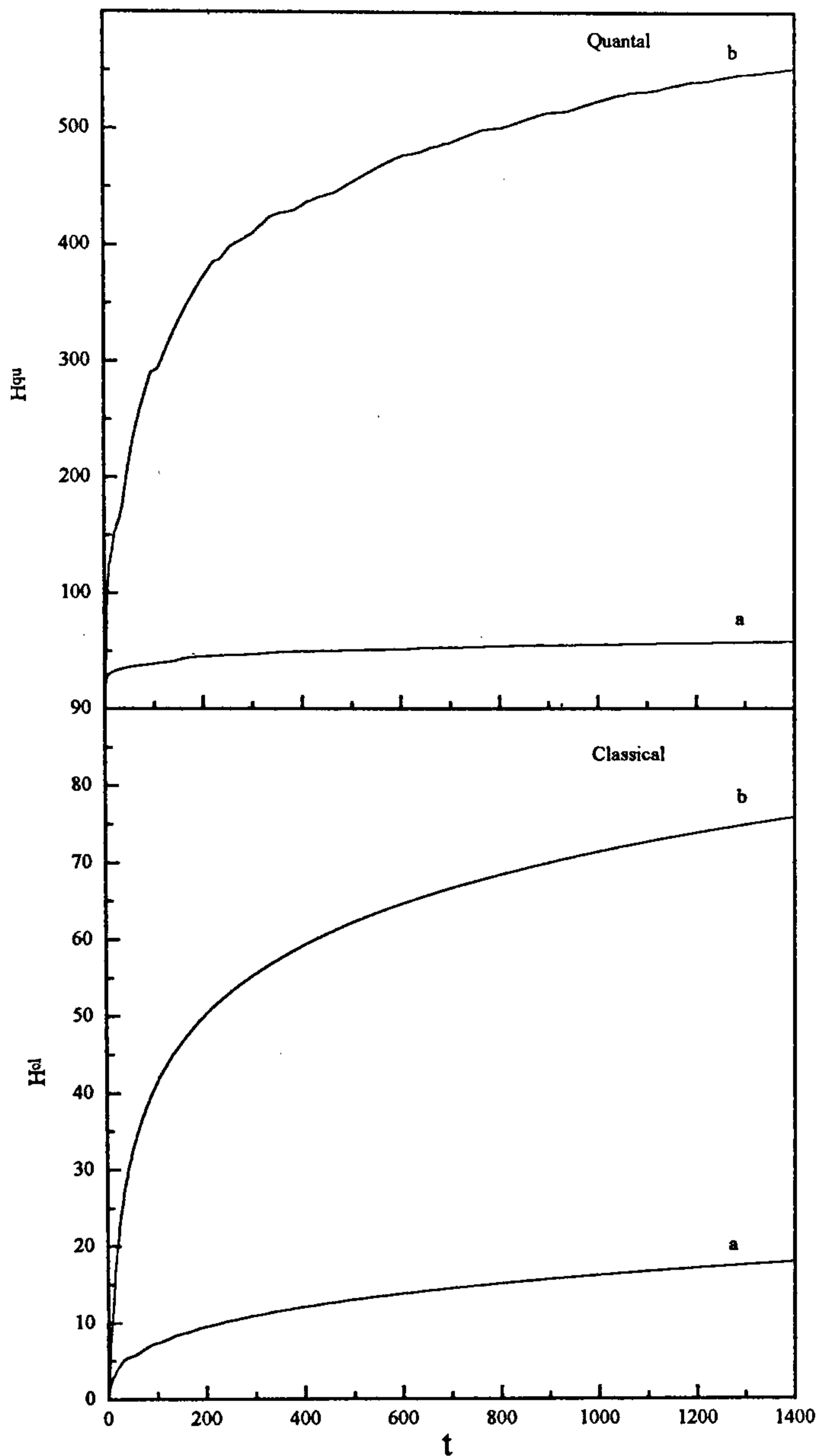


Figure 3. Time evolution of the KS entropy associated with the classical motion (H^{cl}) and quantal motion (H^{qu}) for a double-well oscillator in the presence of an external field with $c = 10$ and two different initial conditions: (a) ($x_0 = -2.0, p_0 = 0.0$); (b) ($x_0 = 2.0, p_0 = 0.0$).

To understand the classical regular/chaotic motion associated with the field-induced barrier penetration in a quartic potential we solve the relevant classical Hamilton's equations of motion using a fourth order Runge-Kutta method. In order to study the corresponding quantum signatures we generate the respective Bohmian trajectories. For this purpose, the numerical solution is launched with the propagation of a Gaussian wavepacket under the influence of the quartic potential (eq. (9)). The details of the numerical solution are available elsewhere^{10,23}. Mesh sizes adopted are $\Delta x = 0.1$ and $\Delta t = 0.02$. Calculation is carried out for $-15 \leq x \leq 15$ and for 10^5 time-steps. It may be noted that the classical phase space

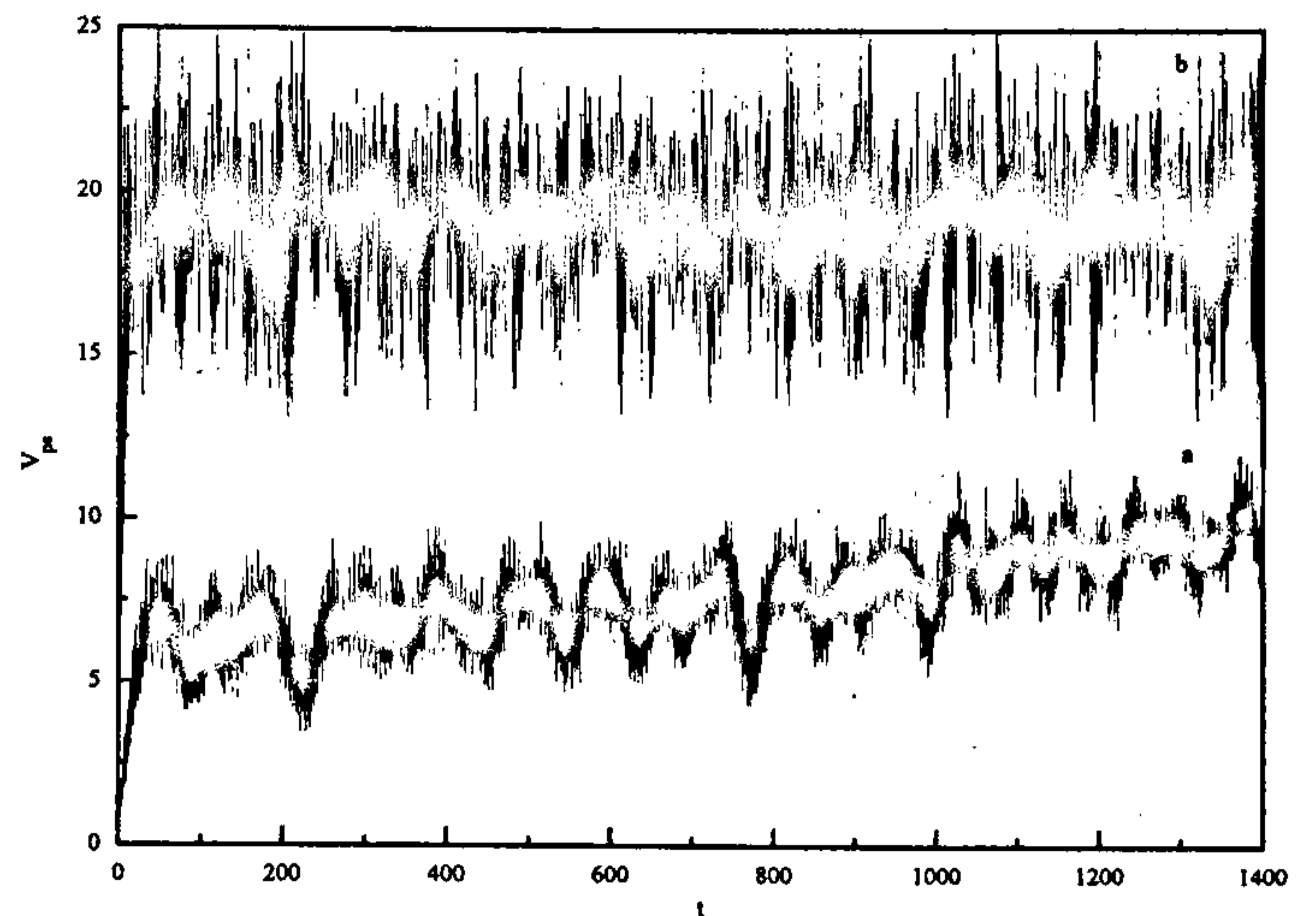


Figure 4. Time evolution of the phase space volume V_{ps} associated with the quantal motion for a double-well oscillator in the presence of an external field with $c = 10$ and two different initial conditions: (a) ($x_0 = -2.0, p_0 = 0.0$); (b) ($x_0 = 2.0, p_0 = 0.0$).

for this problem is three-dimensional (x, p, t) and hence possesses the minimum number of phase space degrees of freedom to exhibit the possible chaotic behaviour. However, momentum is not a 'true variable' in the case of the corresponding quantum system. In the present study, like others⁹⁻¹⁴, we are interested in the signature of the classically chaotic motion, if any, in the associated quantum dynamics.

Once we know $\psi(x, t)$, we can rewrite eq. (3) as:

$$\dot{x} = \nabla \chi(x, t)|_{x=x(t)} = \text{Re} \left[-\frac{i \nabla \psi}{\psi} \right], \quad (10)$$

which has been solved with two different initial conditions (cases (a) and (b)) to obtain the Bohmian trajectories. A second-order Runge-Kutta method is used for this purpose.

In order to understand the breakdown¹⁵ of KAM tori with increasing amplitude of the external field and a possible quantum suppression of the classical chaos, the calculation for case (a) is repeated for two other values of c , viz. 20, 40.

Figure 1 depicts the classical phase space trajectories (stroboscopic plots) for the double-well oscillator in the presence of an external field for two different initial conditions (cases (a) and (b)). While case (a) corresponds to a regular island, case (b) gives rise to the chaotic sea. The KAM torus is surrounded by the following phase-space points, (x, p_x) , in this case: $(-2.00, 0.00)$, $(-1.05, 0.00)$, $(-1.72, -1.65)$ and $(-1.72, 1.65)$.

Corresponding quantal phase portraits generated through the respective Bohmian trajectories are presented in Figure 2. The quantal behaviour properly mimicks the underlying classical dynamics, viz. a regular island for case (a) and a chaotic sea for case (b). It

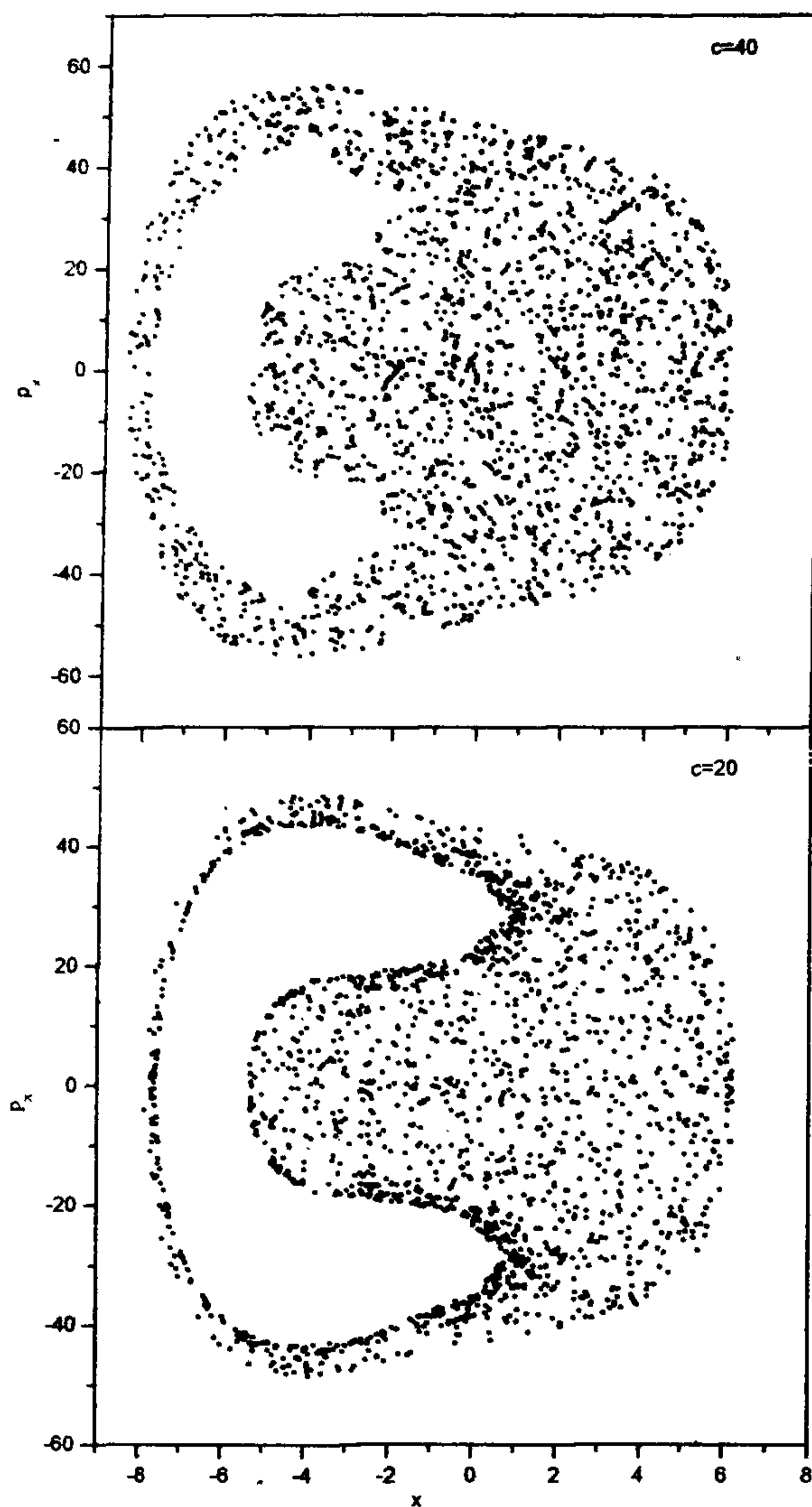


Figure 5. Classical phase space trajectory for a double-well oscillator in the presence of an external field with $c = 20$ and $c = 40$ with initial condition: $(x_0 = -2.0, p_0 = 0.0)$.

appears that a cantor-like structure¹⁶ is a quantum equivalent of the classical KAM torus. The cantor is 'bounded' by the following phase-space points: $(-3.90, 0.00)$, $(-2.00, 0.00)$, $(-3.00, 5.00)$ and $(-3.00, -5.00)$. It is important to note that although the initial conditions associated with classical regular/chaotic behaviour give rise to quantal regular/chaotic behaviour, the size and the position of the classical KAM torus are not necessarily the same as those of the quantal cantor.

Figures 3 and 4 present respectively the classical (H^{cl}) and quantal (H^{qu}) KS entropies and the phase space

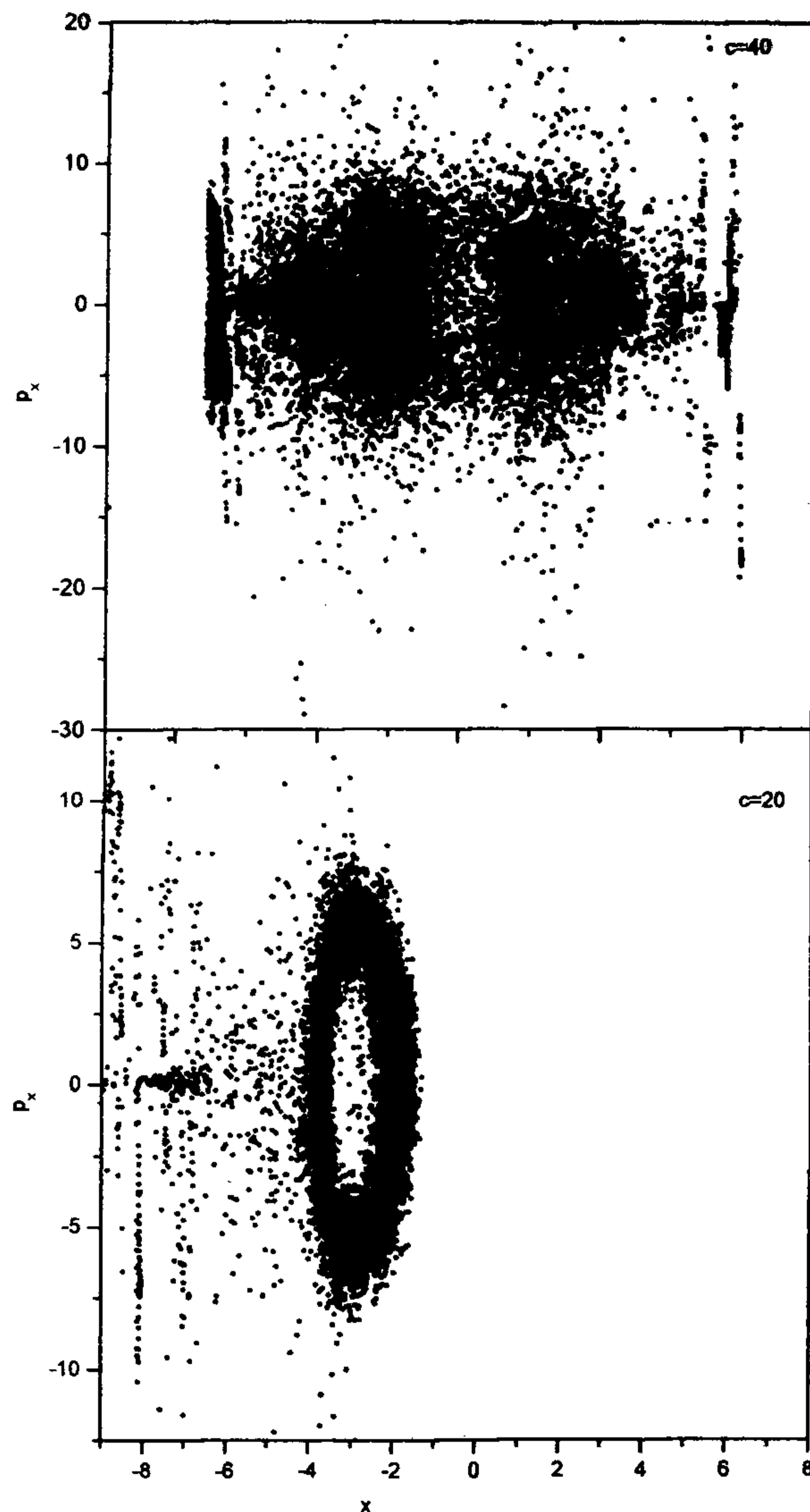


Figure 6. Quantal phase space trajectory for a double-well oscillator in the presence of an external field with $c = 20$ and $c = 40$ with initial condition: $(x_0 = -2.0, p_0 = 0.0)$.

volume (V_{ps}). It may be noted that the orders of magnitude of H^{cl} and H^{qu} are not the same. It is, however, transparent in these plots that the classical stochasticity enhances quantal fluctuations.

In order to investigate the breakdown of the KAM torus¹⁵ (case (a)) when the strength of the perturbation is increased as well as any possible quantum suppression¹⁻¹⁴ of the classical chaos, we study the behaviour of the double-well oscillator in the presence of the external field with two other amplitudes, viz. $c = 20$ and 40 , and the same initial conditions as in case (a) which corresponds to a regular motion for $c = 10$.

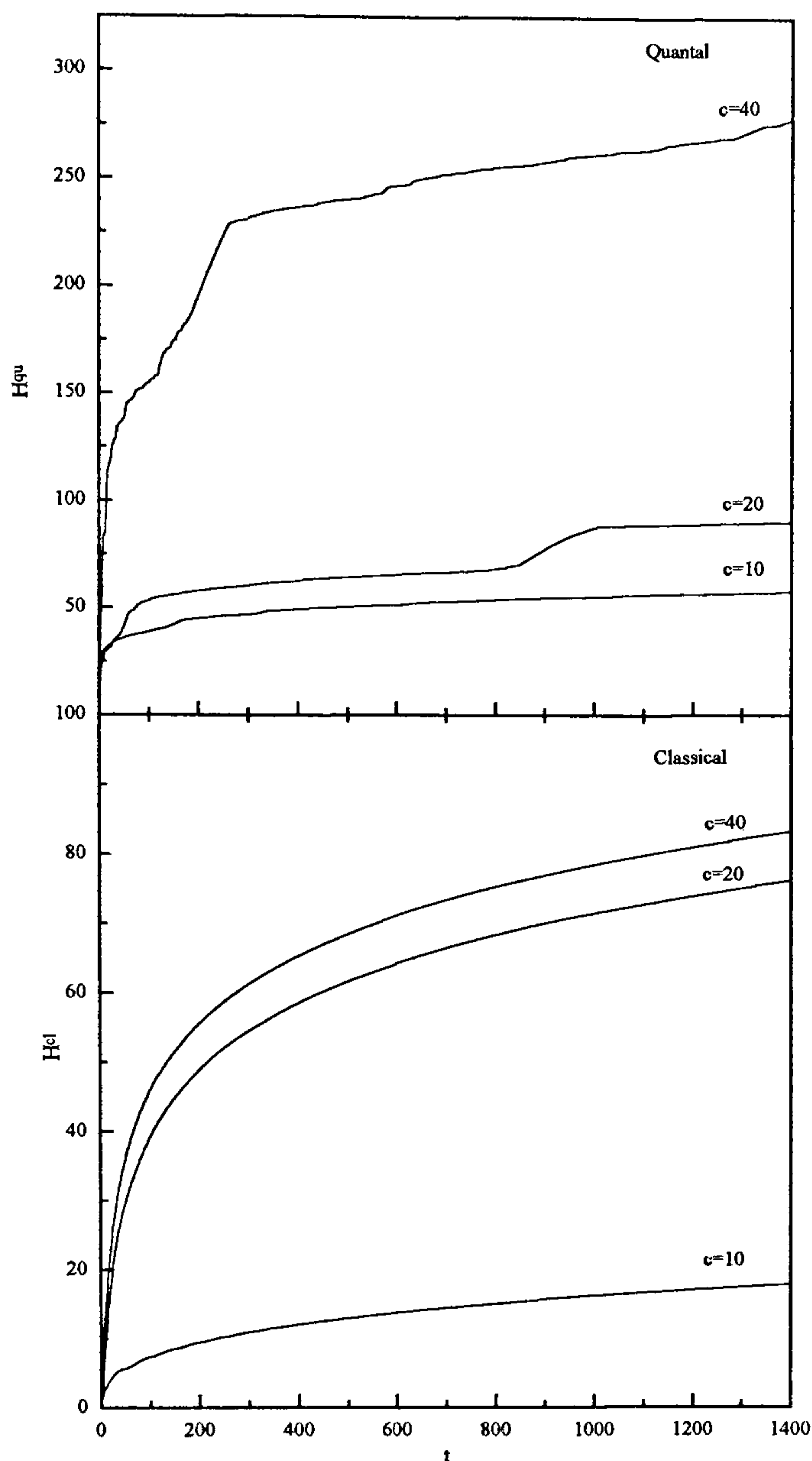


Figure 7. Time evolution of the KS entropy associated with the classical motion (H^{cl}) and quantal motion (H^{qu}) for a double-well oscillator in the presence of an external field with $c = 10, 20$ and 40 respectively, with initial condition: $(x_0 = -2.0, p_0 = 0.0)$.

Figure 5 presents the stroboscopic plots of the classical trajectories for case (a) corresponding to $c = 20$ and $c = 40$, respectively. It is transparent in these plots that the regular island ($c = 10$) is destroyed and the phase space appears to be completely chaotic, more pronounced for the higher c value. Similar plots for the respective quantal motion are given in Figure 6. It is quite clear that a 'cantorus-like' island still persists for $c = 20$ which, however, breaks down for $c = 40$. This fact provides an unmistakable signature of the quantum suppression of chaos. The size and the position of the

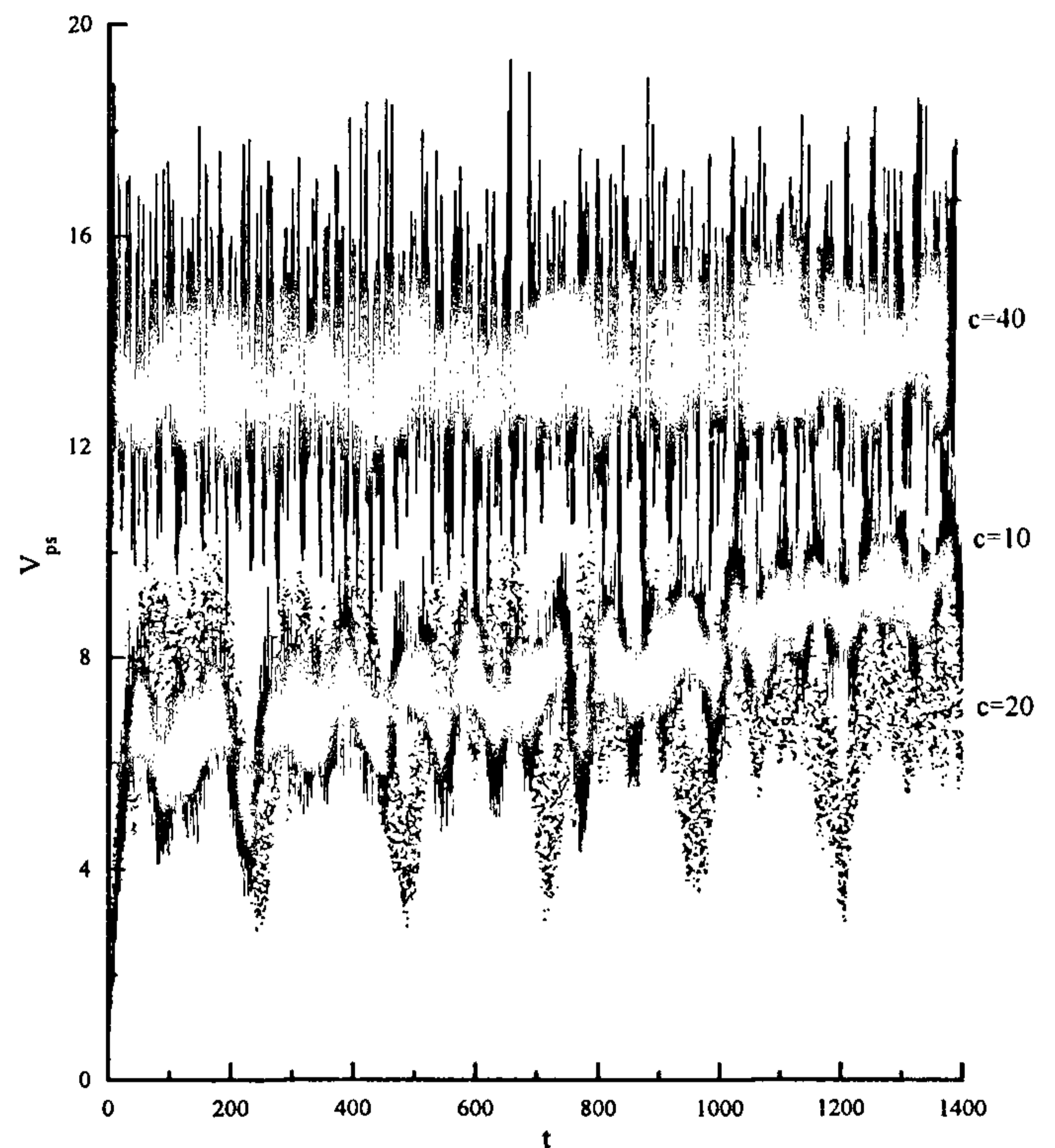


Figure 8. Time evolution of the phase space volume V_{ps} associated with the quantal motion for a double-well oscillator in the presence of an external field with $c = 10, 20$ and 40 respectively, with initial condition: $(x_0 = -2.0, p_0 = 0.0)$.

cantorus ($c = 20$) remain more or less the same as in the case of $c = 10$.

Figure 7 depicts H^{cl} and H^{qu} while Figure 8 presents V_{ps} for the above mentioned cases. These quantities mimic all the trends and strengthen the above inference. For the classical case, H^{cl} remains small for $c = 10$ but increases rapidly for the other two c values. For $c = 10$ and 20 , H^{qu} values are relatively much smaller when compared to the corresponding value for $c = 40$. When the cantorus breaks down ($c = 40$), very large quantum fluctuations are clearly revealed by the V_{ps} plots while the V_{ps} values are comparable for $c = 10$ and 20 .

To summarize, important insights into the quantum manifestations of the classical regular and chaotic motions of a double-well oscillator in the presence of an external field with different amplitudes have been obtained in terms of the corresponding Bohmian trajectories. Two quantum systems which exhibit regular and chaotic motions respectively in the classical domain can be differentiated with the help of the quantum theory of motion. It has been demonstrated for the first time in terms of stroboscopic plots within a Bohmian mechanical framework that the classical chaos enhances the quantum fluctuations and quantum nonclassical effects suppress the classical stochasticity. The KS entropy and phase space volume support this result.

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