Quantum chaos and Hénon-Heiles model: 
Dirac’s variational approach with Jackiw-Kerman function

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A simple semiclassical Hénon-Heiles model is constructed based on Dirac’s time-dependent variational principle. We obtain an effective semiclassical Hamiltonian using a Hartree-type two-body trial wavefunction in the Jackiw-Kerman form. Numerical results show that quantum effects can in fact induce chaos in the non-chaotic regions of the classical Hénon-Heiles model.

1. Introduction

In recent years, interests in classical and quantum chaos have been revived owing to the interesting part they may play in issues such as quantum entanglement, quantum coherence, quantum localization, fast information scrambling, thermalization, etc., in quantum many-body systems (see e.g., Ref.[1-4]), and also in quantum field theory and gravity (see e.g., Ref.[5-9]).

Classical chaos is concerned with the sensitivity of the dynamics of a system to its initial conditions. Two trajectories in phase space whose initial conditions are very close will diverge exponentially in time. The rate of this separation is characterized by the Lyapunov exponent.

In quantum mechanics, the notion of phase-space trajectories loses its meaning owing to the Heisenberg uncertainty principle. It appears that most quantum systems do not exhibit exponential sensitivity and chaos. Still, there are examples of quantum systems that show chaotic behaviors. For instance, the hydrogen atom in a strong magnetic field displays strong irregularities in its spectrum[10] and the wave functions of the quantum mechanical model of the stadium billiard shows irregular patterns.[11] Hence, it is natural to look for quantum manifestations of chaos in classically chaotic systems.[12]

Most research efforts in quantum chaos concerns the quantization of classically chaotic systems in the semiclassical regime. Different approaches have been adopted to identify the signatures of chaos in these quantized systems. The most commonly employed ones are: random matrices,[12-13] energy level dynamics,[13] periodic orbit expansions,[15] Gaussian wave-packet dynamics,[16] etc.
As semiclassical dynamics are generally believed to be qualitatively similar to those of the quantum system and the classical limit of it, so an integrable classical system would not be chaotic in its semiclassical approximation. That is, quantum fluctuations will suppress chaos. However, in [18] it has been demonstrated that this is not always true. Using a semiclassical dynamics derived via the Ehrenfest theorem, the authors showed that for the double-well system, quantum fluctuations may induce chaos. More recently, while we were preparing this manuscript, a new work [19] came to our attention which shows that quantum corrections by metric extensions also favor chaotic behavior in the dynamics of a probe particle near the horizon of a generalized Schwarzschild black hole.

We would like to examine if there are other systems in which chaos could be induced by quantum effects. The example we consider is the Hénon-Heiles model. Originally the Hénon-Heiles potential was used to model the motion of a star in the gravitation field of a galaxy, but later it was found to be also useful as a model of triatomic molecule in quantum chemistry. Thus it becomes of interest to study the quantum behaviors of the Hénon-Heiles model.

It is known that the Hénon-Heiles potential admits both regular and chaotic motions ([see, e.g., Ref. [21-23]). In Ref.[24], by determining the quantum energy levels of the Hénon-Heiles system, it was found that the energy levels in the classically quasi-periodic regime continued smoothly into the classically stochastic regime. Thus quantum fluctuations appear to suppress classical chaos in the Hénon-Heiles potential. More recently, studies of a semiclassical Hénon-Heiles model using the method of Gaussian effective potential also indicate that quantum fluctuations destroy the chaotic behavior in the Hénon-Heiles potential.

In this work, we propose to study a semiclassical Hénon-Heiles model based on Dirac’s time-dependent variational principle [25-28]. In this approach, one first constructs the effective action \( \Gamma = \int dt \langle \Psi(t), t | i\hbar \partial_t - \mathcal{H} | \Psi(t), t \rangle \) for a given system described by a Hamiltonian \( \mathcal{H} \) and a quantum state \( |\Psi(t), t \rangle \) parametrized by some time-dependent \( c \)-variables. Variation of \( \Gamma \) is then the quantum analogue of the Hamilton’s principle. This gives the Hamiltonian equations for the \( c \)-variables. The time-dependent Hartree approximation emerges when a specific ansatz is made for the state \( |\Psi(t), t \rangle \).

For our semiclassical Hénon-Heiles model, we shall assume the two-body state \( |\Psi(t), t \rangle \) to be factorisable into single-particle states described by the Jackiw-Kerman (JK) function [29-31]. With the time-dependent \( c \)-variables in these JK functions, the number of degrees of freedom of the semiclassical system is twice that of the classical one. The new variables could introduce additional nonlinearity into the system. And this may induce chaos in the originally regular regime of the classical system. We investigate such possibility by numerically varying the effective Planck constant (to be defined in Sect. 2) in the effective action. We find that this is indeed the case. Thus, our semiclassical Hénon-Heiles model shows that quantum effects could induce chaos in classically non-chaotic systems.

After this work was submitted, we became aware of Ref. [32], where the same
approach was applied to the study of semiquantum chaos in the one-dimensional double-well oscillator model. The study of this simple model, as explained by the authors, was to serve as a first step towards a better understanding of the (3 + 1)-dimensional scalar Higgs field model. Unlike the Hénon-Heiles model, which admits both regular and chaotic motions, the classical double-well oscillator system behaves regularly. Using as control parameter the total energy of the semiclassical system, determined by the $c$-variables in the initial JK state function, it was also realized that there are energy dependent transitions between regular and semiquantum chaos.

We shall derive in Sect. 2 the effective Hamiltonian of the semiclassical Hénon-Heiles model based on the Dirac’s variational principle. Dynamical behaviors of the corresponding classical model are discussed in Sect. 3, and those of the semiclassical system in Sect. 4. Sect. 5 concludes the paper.

2. The Hénon-Heiles model

The Hamiltonian of the quantum Hénon-Heiles model is

$$H = \frac{1}{2} \sum_{i=1}^{2} \left( \hat{p}_i^2 + \hat{x}_i^2 \right) + \lambda \left( \hat{x}_1^2 \hat{x}_2 - \frac{1}{3} \hat{x}_3^2 \right),$$

where $\hat{x}_i$ and $\hat{p}_i = -i\hbar \partial / \partial x_i$ are the position and momentum operators of the $i$th particle, and $\lambda$ is the coupling strength. To study quantum effects one might vary the Planck constant $\hbar$, but this may leave an uneasy feeling that $\hbar$ is a natural constant and thus cannot be changed. As such, to facilitate numerical analysis, we find it convenient to define the model in terms of the rescaled variables

$$\hat{Q}_i \equiv \lambda \hat{x}_1, \quad \hat{P}_i \equiv \lambda \hat{p}_i = -i\hbar' \frac{\partial}{\partial Q_i}, \quad i = 1, 2,$$

where the effective Planck constant is $\hbar' \equiv \lambda^2 \hbar$. Also we have $H = H' / \lambda^2$ with

$$H' = \frac{1}{2} \sum_{i=1}^{2} \left( \hat{P}_i^2 + \hat{Q}_i^2 \right) + \hat{Q}_1^2 \hat{Q}_2 - \frac{1}{3} \hat{Q}_3^3.$$  

As mentioned in the Introduction, to study quantum effect on the dynamical behavior, especially on the chaotic behavior, of the system, we will construct a semiclassical version of the Hénon-Heiles model. We adopt here the Dirac’s time-dependent variational principle by considering the effective action

$$\Gamma = \int dt \, \langle \Psi, t | i\hbar \partial_t - H | \Psi, t \rangle$$

$$= \frac{1}{\lambda^2} \int dt \, \langle \Psi, t | i\hbar' \partial_t - H | \Psi, t \rangle.$$

We assume the trial wavefunction of the quantum Hénon-Heiles system to have the Hartree form $|\Psi, t \rangle = \prod_i |\psi_i, t \rangle$, where the normalized single-particle state $|\psi_i, t \rangle$ is
taken to be the JK wavefunction:

\[
\langle Q_i|\psi_i, t \rangle = \frac{1}{(2\pi\hbar G_i)^{1/2}} \times \exp\left\{-\frac{1}{2\hbar'} (Q_i - x_i)^2 \left[\frac{1}{2} G_i^{-1} - 2i\Pi_i\right] + \frac{i}{\hbar'} p_i (Q_i - x_i)\right\}.
\] (5)

The real quantities \(q_i(t), p_i(t), G_i(t)\) and \(\Pi_i(t)\) are variational parameters which do not vary at \(t = \pm \infty\). The JK wavefunction can be viewed as the \(Q\)-representation of the squeeze state. We prefer to use the JK form since the physical meanings of the variational parameters in the JK wavefunction are most transparent, as we shall show below. Furthermore, the JK form is in the general Gaussian form so that integrations are most easily performed.

It is not hard to work out the following expectation values:

\[
\langle \Psi|\hat{Q}_i|\Psi \rangle = x_i, \quad \langle \Delta Q_i \rangle = \langle (\hat{Q}_i - x_i)^2 \rangle = \hbar' G_i,
\]
\[
\langle \Psi|\hat{P}_i|\Psi \rangle = p_i, \quad \langle \Delta P_i \rangle = \langle (\hat{P}_i - p_i)^2 \rangle = 4\hbar' G_i \Pi_i^2 + \frac{\hbar'}{4G_i}.
\] (6)

It is clear that \(x_i\) and \(p_i\) are the expectation values of the operators \(\hat{Q}_i\) and \(\hat{P}_i\). Also, \(\hbar' G_i\) is the mean fluctuation of the position of the \(i\)th particle and that \(G_i > 0\). \(\Pi_i\) is related to the mean fluctuation of \(\hat{P}_i\). The uncertainty relation is

\[
\Delta Q_i \Delta P_i = \frac{\hbar'}{2} \sqrt{1 + (4G_i \Pi_i)^2}.
\] (7)

Other expectation values needed to evaluate the effective action are:

\[
\langle \Psi|\hat{Q}_i^2|\Psi \rangle = x_i^2 + \hbar' G_i,
\]
\[
\langle \Psi|\hat{P}_i^2|\Psi \rangle = p_i^2 + 4\hbar' G_i \Pi_i^2 + \frac{\hbar'}{4G_i},
\]
\[
\langle \Psi|\hat{Q}_i^3|\Psi \rangle = x_i^3 + 3\hbar' G_2 x_2,
\]
\[
\langle \Psi|\hat{Q}_i^2 \hat{Q}_2|\Psi \rangle = x_i^2 x_2 + \hbar' G_1 x_2,
\]
\[
\langle \Psi|\hbar' \partial_i|\Psi \rangle = \sum_i (p_i \dot{x}_i - \hbar' G_i \Pi_i).
\] (8)

With these expectation values, the effective action \(\Gamma\) for the Hamiltonian \(H\) can be worked out to be

\[
\Gamma(x, p, G, \Pi) = \frac{1}{\lambda^2} \int dt \left[ \sum_i (p_i \dot{x}_i + \hbar' \Pi_i G_i) - H_{\text{eff}} \right],
\] (9)

where \(H_{\text{eff}} = \langle \Psi|H|\Psi \rangle\) is the effective Hamiltonian given by

\[
H_{\text{eff}} = \frac{1}{2} \sum_{i=1}^2 \left(p_i^2 + x_i^2\right) + x_2^2 x_2 - \frac{1}{3} x_2^3
\]
\[
+ \hbar' \left[\frac{1}{2} \sum_i \left(\frac{1}{4G_i} + G_i + 4G_i \Pi_i^2\right) + (G_1 - G_2) x_2\right].
\] (10)
One sees from the form of the effective action $\Gamma$ that $\Pi_i$ is the canonical conjugate of $\hbar'G_i$. The second line of (10) gives the quantum contribution to the classical Hamiltonian in this semiclassical model.

3. The classical system

From Eq. (10), the Hamiltonian of the classical Hénon-Heiles model is taken to be $H_c \equiv H_{\text{eff}}(\hbar' = 0)$, i.e.,

$$H_c = \frac{1}{2} \sum_{i=1}^{2} (p_i^2 + x_i^2) + x_1^2 x_2 - \frac{1}{3} x_2^3,$$

where $x_i$ and $p_i$ are the position and momentum of the $i$th particle. The Hamiltonian equations of motion are

$$\dot{x}_1 = p_1, \quad \dot{p}_1 = -x_1 - 2x_1 x_2,$$
$$\dot{x}_2 = p_2, \quad \dot{p}_2 = -x_2 - x_1^2 + x_2^2.$$

Here the dot represents derivative with respect to time $t$.

The behavior of this system has been well studied. Fig. 1 depicts the three-dimensional and the contour plot of the potential. It has a three-fold rotational symmetry, is unbounded from below, but has a local minimum in the center within which a particle can be confined. It is found that the system is practically integrable for energy below $E = 1/12 \approx 0.0833$, and as the energy increases the system becomes more and more ergodic, with invariant curves and ergodic regions coexisting, and is completely ergodic at the escape energy $E = 1/6 \approx 0.1667$.

Two commonly used methods to study the behavior of the system are the Poincaré section (or Poincaré surface of section) and the Lyapunov exponent. For Poincaré section, one plots the points of intersection of the orbit of the motion and a two-dimensional plane, here taken to be the $p_2-x_2$ plane with $x_1 = 0$ and $p_1 > 0$. For simplicity, we choose $x_1(0) = x_2(0) = x_0$ and $p_1(0) = p_2(0) = p_0$. The system of equations (12) is solved using a fourth-order explicit Runge-Kutta method with fixed time step size of 0.02, up to total time of 20,000 units.

The Lyapunov exponent $\lambda(t)$ measures how fast two initially nearby orbits are separated as time passes. We shall be interested in the separation of two neighboring orbits in the configuration space. So we define the Lyapunov exponent by

$$\lambda(t) \equiv \frac{\ln d(t) - \ln d(0)}{t},$$

where $d(t)$ is the separation of two nearby initial points in the configuration space at time $t$. The system is said to be chaotic if $\lim_{t \to \infty} \lambda(t) > 0$. We take two nearby initial points $(x_1(0), x_2(0), p_1(0), p_2(0))$ and $(x'_1(0), x'_2(0), p'_1(0), p'_2(0))$ with their separation $d(t) = \sqrt{(x'_1(t) - x_1(t))^2 + (x'_2(t) - x_2(t))^2}$. The two neighboring points are so chosen so that they have the same energy. For illustration purpose, we choose $p_1(0) = p_2(0) = p'_1(0) = p'_2(0)$, and $x'_2(0) = x_2(0) + \Delta x_2(0)$ with $\Delta x_2(0) = 0.0001$. 

Then the condition of equal energy gives 
\[ x'_1(0) = \sqrt{C/(2x'_2(0) + 1)}, \]
where the constant 
\[ C = (2x_2(0) + 1)x_1(0)^2 + (x_2(0)^2 - x'_2(0)^2) - \frac{2}{3}(x_2(0)^3 - x'_2(0)^3). \] (14)

In Figs. 2 we plot the Poincaré sections and Lyapunov exponents for the classical
equation of motion (12) with the initial data
\[ \{x_0, p_0\} = \{0.12, 0.001\}, \{0.10, 0.01\}, \text{ and } \{0.20, 0.01\}, \]
and in Fig. 3 for \( p_0 = 0.01 \) and \( x_0 = 0.30, 0.33, \) and \( 0.35. \) The
corresponding classical energies are:
\[ E = 0.01555, 0.01077, 0.04543, 0.10810, 0.13296 \] and \( 0.15118, \) respectively. One notes that for energies below
\[ E = 1/12 = 0.08333, \]
the Poincaré sections show two invariant curves. The Lyapunov exponents are negative (signaling regular motions), or slightly positive but with regularly appearance
of negative values, indicating that the distance between the two orbits appears to
have some periodic dependence. As the energy becomes higher, such regularity fades
away as ergodicity begins to set in, ergodic regions appear in the Poincaré sections,
and the Lyapunov exponent becomes more positive. Similar behaviors were also
reported in [23].

4. The semiclassical system

Varying the effective action \( \Gamma \) in Eq. (9) with respect to \( x_i, p_i, G_i \) and \( \Pi_i \) then gives
the Hamilton equations of motion in the Hartree approximation:
\[ \dot{x}_i = p_i, \quad \dot{G}_i = 4G_i \Pi_i, \quad i = 1, 2, \]
\[ \dot{p}_1 = -x_1 - 2x_1 x_2; \]
\[ \dot{p}_2 = -x_2 - x_1^2 + x_2^2 - h'(G_1 - G_2), \]
\[ \dot{\Pi}_1 = \frac{1}{8G_1^2} - 2\Pi_1^2 + x_2 - \frac{1}{2}, \]
\[ \dot{\Pi}_2 = \frac{1}{8G_2^2} - 2\Pi_2^2 + x_2 - \frac{1}{2}. \] (15)

This set of equations replaces the classical equations of motion [12].

Our semiclassical model has an extended phase space. To keep our model as close
to the classical model as possible, we choose initial parameters so as to minimize the
quantum effects. From eq. (7), the uncertainty relation is minimal for \( G_i(0) = 0 \) or \( \Pi_i(0) = 0. \) But \( G_i(0) = 0 \) makes the last equation in (6) singular, so we take \( \Pi_i(0) = 0. \) To eliminate initial dependence of \( x_2, \) we take \( G_1 = G_1. \) With these choices, the
quantum part of the initial effective Hamiltonian becomes \( h' \sum_i (G_i + 1/4G_i)/2. \) This
term is minimized with \( G_i = 1/2, i = 1, 2. \) Thus the initial value of the effective
Hamiltonian is \( H_{eff} = E + h', \) where \( E \) is the energy evaluated using only the
classical Hamiltonian \( H_c. \) For \( h', \) we take \( h' < E/10 \) in this work to keep quantum
effect within reasonable bound. Also, the choices \( G_1 = G_2 \) and \( \Pi_i = 0 \) mean that for
the computation of the Lyapunov exponent, we can take the two neighboring initial
points, with the same effective energy, by the same criterion as in the classical case
with the choice [14].
In Figs. 4-7, we plot the Poincaré sections and Lyapunov exponents with different values of $\hbar'$ for the first four sets of $\{x_0, p_0\}$ in Fig. 2 and 3. As discussed in Sect. 3, these sets of parameters give regular classical motions in Hénon-Heiles systems. However, it is obvious that with reasonably small values of $\hbar'$, the distribution of points in the Poincaré section becomes more diffusive and stochastic. The corresponding Lyapunov exponents also become more positive as $\hbar'$ increases. This indicates that, in this semiclassical approximation, quantum effects could induce chaos in classically regular systems.

It is interesting to note that, for large values of $\hbar'$ considered here, the distribution of the points in the Poincaré sections, while appears stochastic, seems to stay in a ring-shaped region.

5. Conclusions

In this work we have attempted to investigate, in the semiclassical approximation, if quantum effects could induce chaos in a classically regular system. The system we considered is the Hénon-Heiles model, which is known to admit both regular and chaotic motions. To construct a semiclassical effective Hamiltonian that incorporates quantum correction, we have employed the Dirac’s time-dependent variational approach with a Hartree-type two-body trial wavefunction in the Jackiw-Kerman form. The effective Hamiltonian is described by the parameters that specified the Jackiw-Kerman wavefunction. Quantum effect on the motion of the system is studied numerically by varying the effective Planck constant in the effective Hamiltonian. Our results show that it is possible for quantum effects to induce chaos in classically non-chaotic systems.

It is noted that the same approach has previously been applied to a one-body double-well oscillator model. The motion of this system is regular classically. Quantum effect on the motion of the semiclassical system was studied using the total energy as the control parameter. It was also shown that the motion of the system can become chaotic due to quantum effect.

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Fig. 1. Three-dimensional and contour plots of the classical Hénon-Heiles potential
Fig. 2. Poincaré sections (left) and Lyapunov exponents (right) for the classical equation of motion with the initial data \( \{x_0, p_0\} = \{0.12, 0.001\}, \{0.10, 0.01\}, \) and \( \{0.20, 0.01\} \) (top to bottom). The corresponding classical energies are: \( E = 0.01555, 0.01077 \) and \( 0.04543 \), respectively.
Fig. 3. Poincaré sections (left) and Lyapunov exponents (right) for the classical equation of motion (12) with the initial data $p_0 = 0.01$ and $x_0 = 0.30, 0.33, 0.35$ (top to bottom). The corresponding classical energies are: $E = 0.10810, 0.13296$ and 0.15118, respectively.
Fig. 4. Poincaré sections (left) and Lyapunov exponents (right) for the semiclassical equation of motion (16) with initial data $x_0^0 = 0$, $p_0^0 = 0.001$, $G_1^1 = G_2^2 = 0.5$, $\Pi_1^1 = \Pi_2^2 = 0$, and various values of $\hbar'$ as indicated.
Fig. 5. Poincaré sections (left) and Lyapunov exponents (right) for the semiclassical equation of motion (16) with initial data $x_0 = 0, p_0 = 0.01, G_1 = G_2 = 0.5, \Pi_1 = \Pi_2 = 0$, and various values of $\hbar'$. 

$N' = 0.000001$

$N' = 0.0003$

$N' = 0.0005$

$N' = 0.001$
Fig. 6. Poincaré sections (left) and Lyapunov exponents (right) for the semiclassical equation of motion (16) with initial data $x_0 = 0$, $p_0 = 0.01$, $G_1 = G_2 = 0.5$, $\Pi_1 = \Pi_2 = 0$, and various values of $\hbar'$ as indicated.
Fig. 7. Poincaré sections (left) and Lyapunov exponents (right) for the semiclassical equation of motion (16) with initial data $x_0 = 0$, $p_0 = 0.01$, $G_1 = G_2 = 0.5$, $\Pi_1 = \Pi_2 = 0$, and various values of $\hbar'$ as indicated.