Chaos in Quantum Cosmology

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Most of the foundational work on quantum cosmology employs a simple minisuperspace model describing a Friedmann-Robertson-Walker universe containing a massive scalar field. We show that the classical limit of this model exhibits deterministic chaos and explore some of the consequences for the quantum theory. In particular, the breakdown of the WKB approximation calls into question many of the standard results in quantum cosmology.

It has been suggested by Hawking [1] that the isotropy and homogeneity of the universe is a natural consequence of the Hartle-Hawking [2] “no-boundary” boundary conditions for the quantum state of the early universe. Testing this idea has proved difficult since a realistic model of the quantum state or wave function of the universe must describe the entire geometry and matter content of the universe. In order to make progress, a number of simple models have been introduced. The most extensively studied model employs a homogeneous and isotropic Friedmann-Robertson-Walker (FRW) spacetime with a minimally coupled massive scalar field. Linde [3] showed that for certain initial conditions this model could lead to exponential expansion of the universe and a successful realisation of the inflationary paradigm.

The FRW-scalar field model has been the work-horse of quantum cosmology. It is the model upon which most of the successes of quantum cosmology are based [4–6], in particular, the breakdown of the WKB approximation calls into question many of the standard results in quantum cosmology. In this letter we describe a problem that complicates the interpretation of these results. We show that the classical trajectories of the model exhibit a form of deterministic chaos known as chaotic scattering [7]. This is a cause for concern since the quantum to classical transition is qualitatively different for chaotic and non-chaotic systems. The problem is particularly pronounced in quantum cosmology since the theory is manifestly semi-classical [8], and since the wavefunction of the universe is interpreted using the WKB approximation [9]. As first pointed out by Einstein [10], the WKB approximation fails if the classical evolution is chaotic.

Considering how much work has been done studying such a simple model, it may seem surprising that the chaotic behaviour went unnoticed. In fact, the fingerprints of chaos can be found in some of the early literature [11,12], but it is only now, with an understanding of chaotic scattering, that we can recognise them as such.

The model in question describes a closed FRW universe with Lorentzian metric

\[ ds^2 = -N^2(t)dt^2 + a^2(t)d\Omega^2 \quad (3) \]

minimally coupled to a scalar field \( \phi \). A fuller description of the model can be found in Ref. [13]. The minisuperspace action is given by \( S = \frac{1}{2} \int (NH/a) dt \) where

\[ H = -\left( \frac{1}{N} \frac{da}{dt} \right)^2 + \left( \frac{a^2}{N} \frac{d\phi}{dt} \right)^2 - V(a, \phi) \quad (2) \]

is the classical Hamiltonian and \( V = -a^2 + m^2a^4\phi^2 \) is the minisuperspace potential. The classical equations of motion that follow from varying \( \phi \) and \( a \) are:

\[ \ddot{\phi} + \frac{3}{a} \dot{\phi} + m^2 \phi = 0 \quad (3) \]

\[ \ddot{a} + 2\phi^2 - m^2 \phi^2 = 0 \quad (4) \]

Here an overdot denotes \( N^{-1}d/dt \). Variation of the lapse \( N \) leads to the constraint \( H = 0 \).

The quantum description employs the “wavefunction of the universe” \( \Psi(a, \phi) \), which obeys the Wheeler-DeWitt equation \( \hat{H}\Psi = 0 \). Adopting a particular factor ordering and changing coordinates to \( u = ae^{-\phi} \) and \( v = ae^\phi \), we find

\[ \left( \frac{1}{4} \frac{\partial^2}{\partial u \partial v} + V(u, v) \right) \Psi(u, v) = 0, \quad (5) \]

where the minisuperspace potential now reads

\[ V(u, v) = uv \left( \frac{m^2}{4} - uv (\ln(v/u))^2 - 1 \right). \quad (6) \]

In order to solve these equations we need boundary conditions. Hartle and Hawking have proposed that, in the Euclidean regime, the universe does not have any boundaries in space or time. The Euclidean version of the Lorentzian metric [14] can be expressed in the form

\[ ds^2 = d\tau^2 + a^2(\tau)d\Omega^2(3). \quad (7) \]

The no-boundary proposal demands that the geometry be compact and the matter fields regular. These conditions restrict the boundary conditions at zero volume \( (\tau = 0) \) to be

\[ a = 0, \quad \frac{da}{d\tau} = 0, \quad \phi = \phi_0, \quad \frac{d\phi}{d\tau} = 0. \quad (8) \]

By integrating the Euclidean action from \( \tau = 0 \) to a nearby point \((a, \phi)\) for large \( \phi_0 \) and applying WKB matching techniques, Hawking [15] obtained the boundary condition \( \Psi = 1 \) along the characteristics \( u = 0 \) and
$v = 0$. We will subsequently question the validity of this procedure. The corresponding classical solutions take the form

$$a \approx (m^2 \phi^2)^{-1/2} \sin((m^2 \phi^2)^{1/2} \tau), \quad \phi \approx \phi_0,$$

(9)

with $\phi_0$ a constant. The Euclidean solution is matched onto the Lorentzian metric \cite{Page} near a totally geodesic spacelike surface $\Sigma = \partial S^1 = S^1$ \cite{Page} where $da/dr = 0$. The rotation to imaginary time is thus accomplished by taking $\tau = \pi/(2m\phi) + it$, leading to the Lorentzian boundary conditions

$$a_0 \approx \frac{1}{m\phi_0}, \quad \dot{a}_0 \approx 0, \quad \phi = \phi_0, \quad \dot{\phi}_0 \approx 0.$$

(10)

Typical Lorentzian solutions see the universe inflate, then enter into a dust filled state where $\phi$ oscillates rapidly, before recollapsing to a final singularity as $\phi \to \pm \infty$ monotonically. In addition to these typical solutions there are an infinite collection of anomalous solutions \cite{Page}. The anomalous solutions expand, then recollapse, then bounce and expand again. The cycle of expansion and collapse may continue indefinitely, or may terminate after a finite number of bounces. One of these bouncing solutions is shown in Fig. 1. Also marked are the lines $V \approx 0$ where the bounces occur, and the line $uv = 1$. It is difficult to track bouncing solutions for more than three of four bounces as they are exquisitely unstable.

In a remarkable paper, Page \cite{Page} conjectured that the anomalous solutions comprise a fractal set of perpetually bouncing universes. What Page described is now known as a strange saddle or strange repellor \cite{Page} - the analog of a strange attractor for non-dissipative chaotic systems.

The unstable periodic orbits partition the space of initial conditions (here just the value of $\phi_0$) according to their outcome. Unless a universe bounces perpetually it must eventually encounter one of the cosmological singularities at $a = 0, \phi = \pm \infty$, corresponding to the lines $u = 0, v = 0$ respectively. We can confirm Page’s conjecture by studying the boundaries between the two attractors $u = 0$ and $v = 0$. We do this by color coding $\phi_0$ according to the outcome; grey for $u = 0$ and black for $v = 0$. The attractor basin boundaries are shown in Fig. 2 for a representative range of $\phi_0$. Each successive strip of “Universe DNA” resolves a small portion of the previous strip. We were able to track the fractal structure over 12 decades in magnification before saturating machine precision.

In the close up views we start to see a third, white outcome occurring. These regions correspond to trajectories that inflate by at least 10 e-folds to produce a “big” universe. A higher cut-off, such as the cosmologically interesting value of 60 e-folds, would produce much the same pictures, but with a smaller white region. The lower cut-off was chosen to keep the numerical integration short. 

It is interesting that trajectories near the bouncing solutions can lead to successful inflation (in the sense of solving the age and flatness problems) without requiring a large initial value for $\phi$. For our choice of $m = 1$, a universe that never bounces requires $\phi_0 > 5.88$ to successfully inflate, while a universe that bounces just once can successfully inflate if $\phi_0 \approx 1.19$. Although the fractal set of perpetually bouncing solutions are countable and thus of zero measure, the collection of universes that bounce at least once is uncountably infinite and of non-zero measure. For example, if we randomly chose an initial value of $\phi$ from the region shown in the upper strip of Fig. 2, a “big” universe is formed about once in every thousand attempts.

The set of unstable periodic solutions can be quantified by its spectrum of multifractal dimensions or by its topological entropy \cite{Page}. Both of these methods provide a coordinate invariant measure of chaos in general relativity \cite{Page}. Here we calculate the topological entropy

![FIG. 1. A bouncing classical trajectory in the $(x, y)$ plane. Also shown are the lines $V(u, v) = 0$ (dashed) and $uv = 1$ (dotted). Here $x = (v - u)/2$ and $y = (v + u)/2$.](image)

![FIG. 2. “Universe DNA”: Zooming in on a boundary.](image)
as it can be found analytically. The topological entropy measures the growth in the number of periodic orbits as their period increases. We quantify the length of an orbit by the number of symbols needed to describe it. To do this we need to introduce a symbolic coding. The most efficient coding we could come up with records the symbol $A$ for each upward crossing of the line $uv = 1$, and the symbol $B$ for each crossing of the $y$-axis. For example, the bouncing trajectory shown in Fig. 1 has the coding $ABABABBBABB$. Applying this recipe to the first four primary orbits shown in Fig. 3 we obtain the codings

$$
\begin{align*}
I &= \overline{AB}, & II &= \overline{ABB}, \\
III &= \overline{ABBb}, & IV &= \overline{ABBbb}.
\end{align*}
$$

(11)

Here the overline denotes a sequence to be repeated. We can develop a recurrence relation for the number of periodic orbits, $N(k)$, with period $k$. Writing $N(k) = P(k) + Q(k)$, where $P(k)$ is the number of period $k$ words ending in $A$ and $Q(k)$ the number ending in $B$, we find

$$
Q(k + 1) = P(k) + Q(k), \quad P(k + 1) = Q(k),
$$

(12)

and $N(2) = 2$. The solution is then $N(k) = (\gamma^{k+1} - \gamma^{-k-1})/\sqrt{5}$, where $\gamma = (1 + \sqrt{5})/2$ is the golden mean. The uncountably infinite set of aperiodic orbits described by Page correspond to orbits with $k = \infty$.

![FIG. 3. The first four primary orbits in the $(x, y)$ plane.](image)

Denoting the number of periodic orbits with lengths less than or equal to $k$ by $N(k)$, we find the strange repellor has a topological entropy of

$$
H_T = \lim_{k \to \infty} \frac{1}{k} \ln N(k) = \ln \gamma.
$$

(13)

Since $H_T > 0$, we can conclude that the dynamics is chaotic. It is interesting to note that the system has a 4-dimensional phase space – the minimum number required for chaos to occur in a Hamiltonian system.

Having established that the classical evolution is chaotic, we can consider possible implications for the quantum theory \[17,18\]. It has been suggested that the wave function of the universe will develop small scale structure if the classical dynamics is chaotic \[19\]. This was demonstrated in Ref. \[19\] by artificially choosing a potential with an infinite number of discontinuities. In the present more realistic model, we have to look elsewhere for the source of fine structure since the potential is completely smooth. Moreover, if we accept the boundary condition $\Psi = 1$, there is no reason to expect small scale structure to develop since the evolution is governed by a linear wave equation with a smooth potential \[20\].

On the other hand, it is clear that the WKB approximation breaks down for our model. This breakdown was independently observed by Shellard \[12\] and Kiefer \[13\]. The WKB approximation seeks to interpret $\Psi$ in terms of classical trajectories according to the decomposition

$$
\Psi = \Psi_+ + \Psi_-, \quad \Psi_{\pm} = \sum_n C_n \exp(\pm i S_n),
$$

(14)

where each phase factor $S_n$ is taken to obey the Hamilton-Jacobi equation $(\nabla S)^2 + V = 0$. The integral curves of $\nabla S$ correspond to classical Lorentzian solutions:

$$
\frac{\partial S}{\partial a} = \pi_a = -\frac{a}{N} \dot{a}, \quad \frac{\partial S}{\partial \phi} = \pi_\phi = \frac{a^3}{N} \dot{\phi}.
$$

(15)

The WKB approximation is valid if the amplitude $C$ varies much more slowly than the phase $S$. There is a conserved current $J_n^\alpha = |C_n^\alpha| \partial_\alpha S_n$ associated with the flux of each WKB wave packet. The flux of a bundle of classical trajectories $F_n = \int J_n^\alpha \epsilon_{\alpha \beta} dx^\beta$ remains constant, regardless of the hypersurface on which it is sampled \[8\].

In order for the flux to be constant, $|C_n|^{2}$ must increase if the bundle of trajectories focuses, and decrease if the bundle defocuses. When classical trajectories cross, a caustic occurs and $|C_n|^{2} \to \infty$. The basic WKB approximation breaks down at a caustic, but an enhanced version continues to hold if the caustic is taken to be the source of a new complex conjugate pair of WKB solutions \[8\]. However, even this enhanced WKB approximation breaks down when the system is chaotic as regions near the unstable periodic orbits contain an infinite fractal set of caustics. The sum over the $\Psi_{\pm}$ pairs spawned in these regions does not converge. In addition to the fractal set of caustics, the strange repellor also produces rapid defocusing of nearby trajectories. This rapid divergence drives $|C_n|^{2}$ rapidly to zero, and the WKB approximation again fails. Both of these effects can be seen in the numerical studies of Refs. \[12,13\].

At this juncture we appear to have a contradiction: solutions of the Wheeler-DeWitt equation with the boundary condition $\Psi = 1$ appear completely benign, despite the classical evolution being chaotic and the WKB approximation breaking down.

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We believe the reason for the apparent contradiction can be traced to the boundary condition for $\Psi$. In deriving the condition $\Psi = 1$, Hawking only included a small subset of the non-singular bouncing universes. This was subsequently criticised by Page [21], who argued that the recollapsing, singular paths would modify Hawking’s result. Shellard [12] attempted to calculate the contribution from these paths using an enhanced WKB approximation, but was thwarted by the caustics that developed near the unstable periodic orbits.

Knowing that the root of the problem lies in the chaotic nature of the classical paths, we can suggest a new approach. We conjecture that the contribution from the perpetually bouncing solutions, and the singular paths in their vicinity, can be found by performing a weighted sum over the multiple instantons that contribute to the bouncing solutions (see Fig. 4). The sum should be weighted by the instability exponent for each periodic orbit. The collection of Euclidean instantons that contribute to the strange repellor can be viewed as a fractal set of spherical “Russian Dolls”, with the radius of each 4-sphere given by $1/(m\phi_0)$ where $\phi_0$ takes all values on the fractal boundary.

![FIG. 4. Some of the Euclidean instantons (solid circles) that contribute to the Lorentzian bouncing solution (dashed line) displayed in Fig. 1.](image)

Our proposal is motivated by Gutzwiller’s approach to quantum chaos. The Gutzwiller trace formula expresses the quantum-mechanical energy levels of a chaotic system in terms of a sum over the classical unstable orbits. By adapting some of the techniques developed to evaluate the Gutzwiller sum, we may be able to properly describe the fractal boundary conditions and subsequent chaos in the wave function. It would be interesting to study how these issues impact other approaches to quantum cosmology, such as Vilenkin’s tunneling proposal [5]. A breakdown in the WKB approximation would complicate the notion of “out-going” wavefunctions used in the tunneling approach.

While our arguments are based on a particular model, in the context of a particular approach to quantum cosmology, the issues we have raised will affect any theory of quantum gravity since all dynamical systems need boundary conditions, and generic dynamical systems are chaotic.

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