Large scale effective theory for cosmological bounces

Martin Bojowald

Institute for Gravitational Physics and Geometry, The Pennsylvania State University,
104 Davey Lab, University Park, PA 16802, USA

An exactly solvable bounce model in loop quantum cosmology is identified which serves as a perturbative basis for realistic bounce scenarios. Its bouncing solutions are derived analytically, demonstrating why recent numerical simulations robustly led to smooth bounces under the assumption of semiclassicality. Several effects, easily included in a perturbative analysis, can however change this smoothness. The effective theory is not only applicable to such situations where numerical techniques become highly involved but also allows one to discuss conceptual issues. For instance, consequences of the notoriously difficult physical inner product can be implemented at the effective level. This indicates that even physical predictions from full quantum gravity can be obtained from perturbative effective equations.

PACS numbers: 98.80.Qc, 04.60.Pp, 98.80.Bp

Our universe, extrapolated backwards in time, gets denser and denser, and eventually reaches such extremes that classical general relativity breaks down. This theoretical limitation is to be solved by a quantum theory of gravity. Since fundamental quantum gravity implies dramatic changes to our understanding of space and time, it can at best provide a non-intuitive, deeply quantum description of the situation where even concepts of time break down. More intuitive pictures can be obtained semiclassically, where the only non-singular way a universe can behave is as a bounce at small volume back to larger scales. Often, models with special, mostly homogeneous, bouncing solutions in detailed descriptions are available, but their genericity or stability under perturbations remains uncertain. Special properties are required for such explicit descriptions which make bounces difficult to generalize in particular to inhomogeneities. In general, one can then only fall back to a fully quantum formulation. Nevertheless, under controlled perturbations bounce scenarios could survive and present crucial insights for cosmological scenarios. A self-consistent analysis of solutions and potential effects of perturbations is made possible by the effective description provided below in the framework of loop quantum gravity.

We first consider the model of a free scalar field $\phi$ in an isotropic cosmology, which will later be seen to play an important role for theoretical changes. The scale factor $a$ of the metric then changes in proper time $\tau$ according to the Friedmann equation $(a^{-1}da/d\tau)^2 = \rho$ (ignoring numerical factors) where $\rho = \frac{1}{2} (d\phi/d\tau)^2$ is the energy density of $\phi$. To quantize canonically we need to introduce canonical variables given by the two pairs $(c, p)$ with $c = da/d\tau$, $|p| = a^2$ and $(\phi, p_{\phi})$ with $p_{\phi} = a^3 d\phi/d\tau$. The variable $p$ can in general take both signs unlike the scale factor $a$ because it also contains information on the orientation of space. Here, however, it is sufficient to assume positive $p$. The Friedmann equation then amounts to a condition between the phase space variables. For a free scalar,

$$\frac{p_{\phi}}{\sqrt{2}} = \pm |cp| = \pm H$$  \hspace{1cm} (1)

is a constant of motion, and we can view $\phi = \sqrt{2t}$ as internal time variable in which the dynamics of the system unfolds given by the Hamiltonian $H$. (The value $p_{\phi}$ then plays the same role as constant energy values in classical mechanics and the sign in (1) selects the direction of time.) A direct canonical quantization is not fully straightforward due to the absolute value in $H = |cp|$. Rather than using a quantization of this operator, one can quantize just $cp$ and restrict states to the positive part of its spectrum. Since $H$ is conserved, it suffices to check for a few initial states in which the semiclassicality condition $\Delta H \ll \langle H \rangle$ for an initial state at large volume. Such states are sharply peaked around $\langle H \rangle$, which can easily be chosen positive. Thus, for such states we can work with a quantization of $H = cp$, dropping the absolute value. Then, using the symmetric operator ordering $\hat{H} = \frac{1}{2}(\hat{c}\hat{p} + \hat{p}\hat{c})$, we are lead to the Schrödinger equation $\partial \psi / \partial t = p \partial \psi / \partial p + \frac{1}{2}\psi$ for a wave function $\psi(p, t)$.

In quantum mechanics, one usually solves first for the wave function $\psi$ and then computes suitable expectation values relevant for measurements. Here, it turns out to be faster and much more powerful to solve for such expectation values directly, using a form of generalized Heisenberg equations of motion. All information in the system is contained in expectation values $\langle \hat{c} \rangle$, $\langle \hat{p} \rangle$ and fluctuations or “n-point functions,” using the language of quantum field theory,

$$G^{a,n} := \langle (\hat{c} - \langle \hat{c} \rangle)^{n-a}(\hat{p} - \langle \hat{p} \rangle)^a \rangle_{\text{symm}}$$  \hspace{1cm} (2)

for integer $n \geq 2$ and $a = 0, \ldots, n$ (using again symmetric ordering). Their Heisenberg-type equations of motion are $\langle \hat{c} \rangle = \langle [\hat{c}, \hat{H}] \rangle / i\hbar = \langle \hat{c} \rangle$, $\langle \hat{p} \rangle = \langle [\hat{p}, \hat{H}] \rangle / i\hbar = -\langle \hat{p} \rangle$ which is easily solved by $\langle \hat{c} \rangle(t) = c_1 e^t$, $\langle \hat{p} \rangle(t) = c_2 e^{-t}$.
To proceed similarly for the $G^{n,n}$, we need one additional ingredient since, e.g., $G^{0,2} = (\hat{c}^2) - (\hat{c})^2$ is not the expectation value of an operator and the commutator $[(\hat{c})^2, \hat{H}]$ is not yet defined. We can simply do so referring to the Leibniz rule to be satisfied for commutators, which gives $[(\hat{c})^2, \hat{H}] / i\hbar = 2\hat{c}[(\hat{c}, \hat{H})] / i\hbar = 2(\hat{c})^2$. By this procedure we have $G^{0,2} = (\hat{c}^2 - (\hat{c})^2, \hat{H}) / i\hbar = 2G^{0,2}$, $G^{1,2} = 0$ and $G^{2,2} = -2G^{2,2}$ as well as similar equations for $G^{n,n}$ for $n \geq 3$. Also this is easily solved by $G^{0,2}(t) = c_3e^{-2t}$, $G^{1,2}(t) = c_4$ and $G^{2,2}(t) = c_5e^{2t}$. Finally, fluctuations are subject to the uncertainty relation

$$G^{0,2}G^{2,2} - |G^{1,2}|^2 \geq \frac{1}{2}\hbar^2 |(\hat{c}, \hat{p})|^2$$

which implies $c_3c_5 \geq \hbar^2/4 + c_2^2$. Our solutions represent wave packets following exactly the classical trajectory with constant relative spread $\Delta p / \langle \hat{p} \rangle = \sqrt{G^{2,2} / \langle \hat{p} \rangle}$.

This model is thus exactly solvable in a very strong sense: we are not just able to obtain wave functions in closed form but the dynamics of all $n$-point functions decouples and allows exact solutions. Such a behavior is realized in usual quantum mechanical systems only for very special solvable systems such as the harmonic oscillator. Its similarity to our system is not accidental since both have quadratic, albeit different, Hamiltonians in canonical variables. Otherwise, non-linear coupling terms between $n$-point functions would result, not allowing analytical solutions. Such coupling terms can easily be seen when, e.g., adding an anharmonic potential $\hat{q}^3$ to the harmonic oscillator. Its expectation value can be written as $\langle \hat{q}^3 \rangle = \langle \hat{p} \rangle^3 + 6\langle \hat{p} \rangle G^{2,2} + 6G^{3,3}$, demonstrating the coupling between $\langle \hat{p} \rangle$ and $G^{2,2}$. Calculating equations of motion as above shows that all of them are now coupled non-linearly. In intuitive terms, the coupling describes how a semiclassical wave packet spreads and deforms, back-reacting on the peak motion given by expectation values.

A free scalar isotropic model thus serves as the analog of the harmonic oscillator (or of a free quantum field theory) in quantum cosmology. This observation is of crucial importance, since such free theories always provide the basis for perturbation theory in the form of effective equations [1, 2]. Before discussing this we will first introduce changes implied by a loop quantization which we have not used so far.

The classical system and the above quantization are singular because vanishing volume $p = 0$ is approached arbitrarily closely by the solutions. Loop quantum gravity implies modifications to the dynamics which lead to bounces provided that one starts (and, in this model, then remains) in the semiclassical regime. This has been studied in detail recently [3], where the semiclassicality condition implied large values of the Hamiltonian $H$. A loop quantization leads to a modified Hamiltonian of the form $f(\hat{p})\sin c \hat{c}$, with a function

$$f(p) \sim \begin{cases} |p|(1 + O(\ell_p^2/p)) & \text{for } |p| > \ell_p^2 \\ |p|^{-n} & \text{for } |p| < \ell_p^2 \end{cases}$$

depending on the Planck length $\ell_p$ and a positive $n$. In such an isotropic context, $f$ is bounded from below by a positive number $\tilde{c}$ in contrast to the classical function $p$. If this is used in an “effective” Hamiltonian $H = f(\hat{p})\sin c$, one can easily see how bounces occur because $\sin c$ is bounded from above such that $p$ cannot become arbitrarily small when it solves the equation $H = f(p)\sin c$ for large constant $H$. Numerical solutions to the resulting equation for wave functions are in fact surprisingly well described by the effective Hamiltonian $p\sin c$: a semiclassical peak follows the effective trajectory very precisely with negligible spread and deformations of the wave packet in “time” $\phi$. This is certainly unexpected for a quantum system where in general wave packets spread quickly and move away from the classical trajectory. Our analytical solutions below will explain this behavior and prove the genericity of semiclassical bounces beyond what is possible in a numerical analysis. Unlike previous investigations, the systematic theory is well suited to a perturbation analysis which can be performed even if strong model-specific assumptions are relaxed. It thus provides the technology for developing realistic bounce scenarios.

The expression $p\sin c$, using $f(p) \sim p$ for $p > \ell_p^2$ which as we will see is always the case for our solutions, is not quadratic in the variables $(c, p)$ in contrast to the classical Hamiltonian. This seems to remove the solvability observed before, as it generally happens when solvable Hamiltonians are modified. We are forced to use a different Hamiltonian since the loop quantization does not allow one to act with $c$ itself but only with the exponents $e^{\pm ic}$ appearing in the sine. To deal with the new Hamiltonian, we notice that $H$ can be reformulated in new variables $p$ and $J := pe^{ibc}$ such that a way that it becomes even linear. We then have $H = -\frac{1}{2}(J - \bar{J})$ for a Hamiltonian in non-canonical variables $(J, p)$ with Poisson relations \{ $p, J \} = -i\hbar$, \{ $\bar{p}, J \} = i\hbar$, \{ $J, \bar{J} \} = 2ip$. Thus, the Hamiltonian with these new variables forms a linear algebra isomorphic to sl(2, $\mathbb{R}$). Classical equations of motion can easily be solved, also taking into account the reality condition $JJ = p^2$ for our complex variables.

If such a system remains linear after quantization, it allows a decoupling of the infinitely many quantum variables to finitely many coupled linear equations just as Hamiltonians quadratic in canonical variables do. This would again make exact solutions possible. Quite surprisingly, the loop quantization $H = -\frac{1}{2}(\hat{J} - \hat{\bar{J}})$ with basic commutation relations $[\hat{p}, \hat{J}] = \hat{h}\hat{J}$, $[\hat{p}, \hat{\bar{J}}] = -\hat{h}\hat{\bar{J}}$ and $[\hat{J}, \hat{\bar{J}}] = -2\hbar\hat{q} = h^2$ does remain a linear system.

(These relations follow if the ordering $\hat{J} = \hat{p}e^{ibc}$ is understood.) The classical algebra is simply modified by a
Although central extension of charge $\hbar$. In a quantum theory, there is an additional condition requiring that real variables are promoted to self-adjoint operators. Such conditions determine the physical inner product used to normalize wave functions. We do not use real variables, but the reality condition for $J = pe^{\epsilon t}$ implies $\hat{J}\hat{J} = \hat{p}^2$ to be imposed (but note $\hat{J}\hat{J} \neq \hat{p}^2$ in our ordering). Imposing the reality condition at the quantum level, which can easily be done for quantum variables as we will see below, corresponds to requiring that the physical inner product is used to normalize wave functions.

Proceding as before, we derive generalized Heisenberg equations from commutators. This results in equations of motion $\langle \hat{p} \rangle' = -\frac{1}{\hbar}\left(\langle \hat{J} \rangle' + \langle \hat{J} \rangle \right)$ and $\langle \hat{J} \rangle' = -\langle \hat{p} \rangle - \frac{\hbar}{2} = \langle \hat{J} \rangle$ while $\langle \hat{J} \rangle - \langle \hat{J} \rangle = 2i\hbar$ is constant (where $H = \langle \hat{H} \rangle$). The general solution

$$\langle \hat{p} \rangle(t) = \frac{1}{2}(c_1 e^{-t} + c_2 e^t) - \frac{1}{2}\hbar$$

$$\langle \hat{J} \rangle(t) = \frac{1}{2}(c_1 e^{-t} - c_2 e^t) + iH$$

diffs from that obtained without a loop quantization and exhibits bouncing solutions (for $c_1 c_2 > 0$) and singular ones ($c_1 c_2 < 0$). These solutions still need to be restricted by the reality condition $\hat{J}\hat{J} = \hat{p}^2$. Taking expectation values, this tells us

$$|\langle \hat{J} \rangle|^2 - (\langle \hat{p} \rangle + \frac{\hbar}{2})^2 = \frac{1}{4}\hbar^2 + G - G^{2,2}$$

where we introduced the dispersion variables $G^{2,2} = \langle \hat{p}^2 \rangle - (\hat{p})^2$ and $G = \frac{1}{2}(\hat{J}\hat{J} + J^2) - |J|^2 = \langle \hat{J}\hat{J} \rangle - |J|^2 + \hbar p + \frac{\hbar}{2}e$, using the commutation relations. As before, one can compute equations of motion for the dispersions and verify that the combination $G - G^{2,2} = \epsilon$ is constant in time. This implies a condition for the constants in our solutions $p(t)$ and $J(t)$:

$$|\langle \hat{J} \rangle|^2 - (\langle \hat{p} \rangle + \frac{\hbar}{2})^2 = -4c_1 c_2 + 4\hbar^2 - \epsilon + \hbar^2/4.$$

Since $\epsilon$ is a fluctuation term, it is small for semiclassical states, in which case $c_1 c_2 = H^2 + \frac{\epsilon}{4} - \frac{1}{16}\hbar^2$ is positive. In this case, ignoring small contributions from $\epsilon$ and $\hbar$, only bouncing solutions

$$\langle \hat{p} \rangle(t) = H \cosh(t - \delta), \quad \langle \hat{J} \rangle(t) = -H(\sinh(t - \delta) + i)$$

with $\epsilon^3 := c_1 / H$ remain. Reality conditions of the effective theory thus prove that all solutions which are semiclassical at least one time are bounded away from the classical singularity at $p = 0$. (Note that this property of $\epsilon \ll H^2$ is stronger than the condition $\Delta H \ll H$ imposed to take into account positivity of the Hamiltonian. There are thus physical solutions with large dispersions which reach the classical singularity, and the fact that states which are semiclassical at one time do not reach a singularity is non-trivial.)

Similarly, we can explicitly determine the spread parameters. We use the second order variables $G^{0,2} = \langle \hat{J}\hat{J} \rangle - \langle \hat{J} \rangle^2, G^{1,2} = \frac{1}{2}(\langle \hat{p}\hat{J} \rangle + \langle \hat{J}\hat{p} \rangle) - \langle \hat{p} \rangle \langle \hat{J} \rangle$ and $G^{2,2} = \langle \hat{p}^2 \rangle - (\langle \hat{p} \rangle)^2$. (The operator $\hat{J}$, although it appears in the Hamiltonian, is not included in quantum variables here since we can use the commutation relations and the reality condition to express any expectation value containing $\hat{J}$ through quantum variables of the same or lower order not containing $\hat{J}$.) By the general scheme we have equations of motion $G^{0,2} = -2G^{1,2}, G^{1,2} = \frac{1}{4}G^{0,2} - \frac{1}{4}G^{2,2} - \frac{1}{16}\hbar^2, G^{2,2} = -2G^{1,2}$. Thus, $G^{0,2} = G^{2,2} = 2c_3$ is constant while

$$G^{2,2} = \frac{1}{2}(c_4 e^{-2t} + c_5 e^{2t}) - \frac{1}{2}c_3 - \frac{1}{16}\hbar^2$$

$$G^{1,2} = \frac{1}{2}(c_4 e^{-2t} - c_5 e^{2t}).$$

The constants $c_i$ are restricted again by the uncertainty relation which now, in non-canonical variables, reads

$$G^{0,2}G^{2,2} - |G^{1,2}|^2 \geq \frac{1}{4}\hbar^2|\hat{J}|^2.$$  

(9)

For $t \to \pm \infty$, this is easy to evaluate and satisfied only if $c_3, c_4$ and $c_5$ are positive. Moreover, assuming $H \gg \hbar$ and near saturation before as well as after the bounce one has $c_4 e^{-2t} \approx \hbar H \approx c_5 e^{2t}$. With this,

$$|\Delta p(t)|^2 = G^{2,2}(t) \approx \hbar H\cosh(2(t - \delta))$$

(10)

and not only the peak trajectory but also the spread of the wave packet is symmetric around $t = \delta$. But only under the two stated conditions does the solution automatically become as coherent after the bounce as it was before (Fig. 1).

![Graph](https://via.placeholder.com/150)

**FIG. 1:** Peak trajectory with surrounding area spread out by $\Delta p$ around a bounce for $H = 10\hbar$. Dashed lines show the general behavior not assuming uniform spread. This figure is to be compared with the numerical solution in Fig. 2 of [4].

Our solutions in the given ordering are exact [20] quantum solutions where $\langle \hat{p} \rangle(t)$ is unaffected by spreading. This shows clearly why the naive effective formulation, obtained by simply replacing $c^2$ by $\sin^2 e$ in the classical
Hamiltonian, agrees so well with numerical simulations of a related free scalar model [6]. But the smoothness and symmetry of the bounce requires additional assumptions which brings us to its robustness. As mentioned, the model is fully analogous to the harmonic oscillator as far as the decoupling of all its quantum variables is concerned. Using exclusively one solvable model to draw conclusions for the quantum nature of the big bang can then be as misleading as using the harmonic oscillator to determine the general behavior in quantum mechanics would be. Under any new ingredient to make the model more realistic coupling terms between all variables will arise. States then do spread and deform with complicated non-linear back-reaction on the expectation values. We thus need to discuss the expected more general behavior, before coming to effective theory as a means to study stability and develop realistic scenarios.

There are several examples for generalizations. First, while $H \gg \hbar$ is necessary for a semiclassical state at large volume of a homogeneous universe with large matter content, several effects in inhomogeneous models remove this condition. Then, $H$ is a spatial function and its local values relevant for loop variables can be small even with a large matter content. (See [8, 9] for properties of inhomogeneous states and operators defined in a regime around a homogeneous reference metric.) Moreover, with many more degrees of freedom, inhomogeneous situations allow the emergence of a semiclassical state at large volume, e.g. through decoherence, even though the state around the bounce can be highly non-semiclassical. This will complicate an analysis based only on the condition that the universe be semiclassical at one late time.

But already in homogeneous models, several new effects can arise if $H$ is not large, as in those inhomogeneous cases. The bounce scale will be smaller and quantum corrections to the $p$-dependence of the constraint through the function $f(p)$ will appear. Since these corrections are higher powers in $p$, coupling terms between $p$ and all quantum variables arise. At some point, due to the boundedness of $f(p)$, no bounce occurs at all when $H$ is small enough. (A similar removal of the bounce due to structural modifications to the equations, loosely related to potential consequences of inhomogeneous states on small scales, has recently been explored in [10].) Moreover, the behavior becomes more sensitive to the factor ordering of the constraint. Ordering all $\hat{p}$ to the right, for instance, leads to an additional contribution $\hbar^{-1} \hat{J}$ to the constraint. This is of the order $\hbar$ and would not change the above analysis much when $H$ is large, but it does become relevant for smaller $H$. It implies coupling terms of the form $-\hbar G^{1/2} / (\hat{p})^2$. In addition, there are corrections if model specifics are changed. Adding a cosmological constant or positive curvature adds coupling terms to the Hamiltonian, but near the bounce they are not dominant. A potential for the scalar field, however, is more crucial because it leads to a time-dependent Hamiltonian.

In particular the latter change can have strong implications depending on the form of the potential (see, e.g., the last example in [11]). The most important ingredient to introduce is inhomogeneities and their evolution, at least as perturbations around a large isotropic background, which is necessary both for a stability analysis and for cosmological predictions. Inhomogeneities add not only new degrees of freedom but also additional coupling terms between the variables. All this is difficult to analyze numerically, and generalized Heisenberg equations as used here can also become complicated to solve exactly. But all these changes are straightforwardly implemented in a general perturbation scheme around the solvable free scalar model identified here. The model behavior is valid when only large semiclassical scales are involved and interactions are negligible, but it receives corrections when smaller scales are reached or interactions introduced. The resulting picture, accessible perturbatively, can be quite different from the smooth bouncing solutions obtained for large $H$ and isotropic states.

This is not surprising because inhomogeneous situations provide many degrees of freedom over which excitations can be distributed which happens in particular close to a classical singularity. The generic behavior is then different from an isotropic bounce, an observation which has also been made in the context of string theory [12]. General singularity resolution can be achieved by mechanisms taking into account deep quantum behavior which does not necessarily provide intuitive pictures [13, 14, 15, 16]. While such a direct quantum analysis is difficult in explicit terms, effective theory does make it feasible by perturbing around an exact model. Given a Hamiltonian $H = H_0 + H_1(p, J; t)$ with the solvable one $H_0$ and possibly time (i.e., scalar field) dependent coupling terms $H_1$, we find perturbative solutions $\langle \hat{p}(t) | p_0(t) + p_1(t) \rangle$ where $p_0$ is a free solution as above and $p_1$ is obtained by integrating

$$\dot{p}_1 = -i\hbar^{-1} \langle [\hat{p}, \hat{H}_1] \rangle |_{\hat{p} = p_0(t), \hat{J} = J_0(t), G^{a,n} = G_0^{a,n}(t)} .$$

The right hand side is known in terms of zero order solutions. This procedure agrees with perturbation expansions in the interaction picture of quantum field theory. Indeed, effective equations derived by perturbation theory around our solvable model are in complete analogy with low energy effective actions in particle physics [1, 2].

We thus provide the first systematic scheme for a well-defined evolution of perturbations through bounce. It allows us to approach the strong quantum regime and to determine if a semiclassical description would break down. One can, for instance, start with large $H$ and then decrease its value to see corresponding changes in the wave function. (Although different in its nature, this parameter thus plays a role similar to others which have already been used in loop quantum cosmology [17].)
While the parameter should not be large for realistic inhomogeneous bounces, it provides a technical tool to separate some quantum effects from others.) In perturbation theory one can then deal with quantum corrections arising from several coupling terms which may be present.

Effective theory is thus a powerful tool where direct numerical simulations become more involved. One can obtain directly quantities of interest such as expectation values and fluctuations without taking the “detour” of wave functions. What is particularly interesting for full quantum gravity is that even conceptual issues can be addressed. The problem of time does not arise because one is perturbing around a model which is explicitly parameterized. Similarly, observables can be evaluated perturbatively. Even the notoriously difficult issue of the physical inner product, i.e. the issue of how to select normalizable wave functions, can be addressed at the effective level as already seen: we used reality conditions to select the physically viable effective solution which turned out to be bouncing. This corresponds to the correct normalizable wave function [6]. This solution is uniquely selected by referring only to quantum variables side-stepping explicit states, an observation which is encouraging for effective developments in full quantum gravity. In effective equations, one can then implement the physical inner product order by order on effective solutions. In particular, this argument applied to general dynamical expressions provides the strongest indication so far that repulsive effects which have been observed throughout loop cosmological models [19] are active even in a full setting. Although they are not strong enough to lead to general bounces at smaller scales of generic states, we have shown that perturbative regimes of inhomogeneous bounces do exist. Whether or not this is sufficient for our universe can be tested in detailed analyses which are now being undertaken. Through effective theory, all issues relevant for physical predictions can thus be addressed.

Acknowledgements: The author thanks A. Ashtekar, T. Pawlowski and P. Singh for discussions. This work was supported by NSF grant PHY0554771.

* Electronic address: bojowald@gravity.psu.edu
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[20] We had to drop the absolute value of ˆH to derive those solutions, which is well justified for the states we consider here. If there were coupling terms between expectation values and dispersions on the other hand, the semiclassical dynamics would change considerably.