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## Hamiltonian formulation of the Belinskii-Khalatnikov-Lifshitz conjecture

Abhay Ashtekar, Adam Henderson, and David Sloan
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# A Hamiltonian Formulation of the BKL Conjecture 

Abhay Ashtekar ${ }^{1},{ }^{*}$ Adam Henderson ${ }^{1},^{\dagger}$ and David Sloan ${ }^{1,2 \ddagger}$<br>${ }^{1}$ Institute for Gravitation and the Cosmos, Physics Department, Penn State, University Park, PA 16802, U.S.A.<br>${ }^{2}$ Institute for Theoretical Physics, Utrecht University, The Netherlands.

The Belinskii, Khalatnikov and Lifshitz conjecture [1] posits that on approach to a space-like singularity in general relativity the dynamics are well approximated by 'ignoring spatial derivatives in favor of time derivatives.' In [2] we examined this idea from within a Hamiltonian framework and provided a new formulation of the conjecture in terms of variables well suited to loop quantum gravity. We now present the details of the analytical part of that investigation. While our motivation came from quantum considerations, thanks to some of its new features, our formulation should be useful also for future analytical and numerical investigations within general relativity.

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## I. INTRODUCTION

Originally formulated in 1970, the Belinskii-Khalatnikov-Lifshitz (BKL) conjecture states that as one approaches a space-like singularity, 'terms containing time derivatives in Einstein's equations dominate over those containing spatial derivatives' [1]. This implies that Einstein's partial differential equations are well approximated by ordinary differential equations (ODEs), whence the dynamics of general relativity effectively become local and oscillatory. The time evolution of fields at each spatial point is well approximated by that in homogeneous cosmologies, classified by Bianchi [3]. The simplest of these are the Bianchi I metrics which have no spatial curvature and the Bianchi II metrics which have 'minimal'

[^0]spatial curvature. According to the BKL conjecture, the dynamics of each spatial point follow the 'Mixmaster' behavior -a sequence of Bianchi I solutions bridged by Bianchi II transitions. Finally, with the significant exception of a scalar field, matter contributions become negligible - to quote Wheeler, "matter doesn't matter".

In the beginning, the conjecture seemed to be coordinate dependent and rather implausible. However, subsequent analysis by a large number of authors has shown that it can be made precise and by now there is an impressive body of numerical and analytical evidence in its support [4]. It is fair to say that we are still quite far from a proof of the conjecture in the full theory. But there has been outstanding progress in simpler models. In particular, Berger, Garfinkle, Moncrief, Isenberg, Weaver and others showed that, in a class of models, as the singularity is approached the solutions to the full Einstein field equations approach the 'Velocity Term Dominated' (VTD) ones obtained by neglecting spatial derivatives [4-8]. Andersson and Rendall [9] showed that for gravity coupled to a massless scalar field or a stiff fluid, for every solution to the VTD equations there exists a solution to the full field equations that converges to the VTD solution as the singularity is approached, even in the absence of symmetries. These results were generalized to also include $p$-form gauge fields in [10]. In these VTD models the dynamics are simpler, allowing a precise statement of the conjecture that could be proven. In the general case, the strongest evidence to date comes from numerical evolutions. Berger and Moncrief began a program to analyze generic cosmological singularities [11]. While the initial work focused on symmetry reduced cases [12], more recently Garfinkle [13] has performed numerical evolution of space-times with no symmetries in which, again, the Mixmaster behavior is apparent. Finally, additional support for the conjecture has come from a numerical study of the behavior of test fields near the singularity of a Schwarzschild black hole [14].

With growing evidence for the BKL conjecture, it is natural to consider its implications to quantum gravity. The conjecture predicts a dramatic simplification of general relativity near space-like singularities, which are precisely the places where quantum gravity effects are expected to dominate. A promising approach to analyze this issue is provided by loop quantum cosmology (LQC) [15] where there are now several indications that the quantum gravity effects become important only when curvature or matter density are about a percent of the Planck scale. Therefore it is quite possible that, generically, spatial derivatives become negligible compared to the time derivatives already when the universe is sufficiently classical.

In this case a quantization of the effective theory with ODEs, that descends from techniques applicable in the full theory, could provide a reliable qualitative picture of quantum gravity effects near generic space-like singularities. If, on the other hand, the BKL behavior sets in only in the Planck regime, this strategy would not be viable. But since there is no reason to trust Einstein's equations in this regime, then the conjecture would also not have a physically interesting domain of validity.

LQC is the result of application of the principles of loop quantum gravity (LQG) [16-18] to symmetry reduced cosmological models. Initial study of the $\mathrm{k}=0$ Friedmann Lemaitre Robertson Walker (FLRW) models revealed that the quantum geometry effects underlying LQG provide a natural mechanism for the resolution of the big bang singularity [19]. Subsequent more complete analysis led to a detailed understanding of the physics in the Planck regime and also showed that although these effects are very strong there -capable of replacing the big bang with a quantum bounce - they die extremely rapidly so as to recover general relativity as soon as the curvature falls below Planck scale [20]. These results were then extended to include spatial curvature in [21] and a cosmological constant in [22]. More recent investigations reveal that if matter satisfies a non-dissipative equation of state $P=P(\rho)$, LQC resolves all strong curvature singularities of the FLRW models, including, e.g., those of the 'big-rip' or 'sudden death' type [23]. Also, it is now known in LQC that the Bianchi I and II and IX singularities are resolved [24-26].

In view of the BKL conjecture, these results, together with further support from the 'hybrid' quantization of Gowdy models [27], suggest that there may well be a general theorem to the effect that all space-like singularities of the classical theory are naturally resolved in LQG. However, it is difficult to test this idea using the current formulations of the BKL conjecture since these approaches are motivated by the theory of partial differential equations rather than by Hamiltonian or quantum considerations (See e.g., [28, 29]. In particular, most approaches perform a rescaling of their dynamical variables by dividing by the trace of the extrinsic curvature. It is difficult to promote the resulting variables to operators on the LQC Hilbert space. In the analysis presented here, we reformulate the BKL conjecture in a way better suited to LQC and explore the resulting system both analytically and numerically.

In LQG one begins with a first order formalism where the basic canonical variables are a density-weighted triad and a spin-connection [16-18]. In section II we will begin by recalling this Hamiltonian formulation of general relativity. In section III we rewrite this theory using
a set of variables that are motivated by the BKL conjecture. Rather surprisingly, the core of this theory can be formulated using (density weighted) fields with only internal indices; space-time tensors never feature! To understand the implications of the BKL conjecture to LQG, we need to express the conjecture using this Hamiltonian framework. This task is carried out in section IV. We provide a weak and a strong version of the conjecture. The key idea is to say that, as one approaches space-like singularities, the exact system is well approximated by a truncated system which features only time derivatives. Nontriviality of the formulation lies in the choice of variables and specification of how limits are taken. Our procedure satisfies a number of stringent requirements. In particular, one can either first truncate the Hamiltonian and then obtain the equations of motion or first obtain the full equations of motion and then truncate them; the two procedures commute. In section V we study the truncated Hamiltonian system and explore its dynamics in some detail. We show that it exhibits all the known features such as the 'u-map' and spikes. Thus, the Hamiltonian framework we were led to by $L Q G$ considerations successfully captures the Mixmaster dynamics faithfully. Therefore, in addition to providing a viable point of departure to analyzing the fate of generic space-like singularities in LQG, it should also be useful in analytical and numerical investigations of the BKL conjecture in classical general relativity itself. In section VI we summarize the main results and comment on their relation to those of other works.

The two appendices contain more technical material. Appendix A introduces densities in a coordinate-free manner. This notion is important because the basic variables in our formulation of the BKL conjectures are scalar densities of weight 1. In the main text, for simplicity we have set the shift and the Lagrange multiplier of the Gauss constraint equal to zero. Appendix B contains the full equations without these restrictions.

## II. PRELIMINARIES

We will consider space-times of the form ${ }^{4} M=\mathbb{R} \times{ }^{3} M$ where ${ }^{3} M$ is a compact, oriented 3-dimensional manifold (without boundary). ${ }^{1}$ We will formulate general relativity in terms

[^1]of first order variables, the point of departure of LQG [30]. These consist of pairs of fields consisting of a (density weighted) orthonormal triad, $\tilde{E}_{i}^{a}$ and its conjugate momentum $K_{a}^{i}$ which on solutions will correspond to extrinsic curvature. The fundamental poisson bracket is given by
\[

$$
\begin{equation*}
\left\{\tilde{E}_{i}^{a}(x), K_{b}^{j}(y)\right\}=\delta_{i}^{j} \delta_{b}^{a} \delta^{3}(x-y) \tag{2.1}
\end{equation*}
$$

\]

Herein, early letters, $a, b, c$ denote spatial indices while $i, j, k$ denote internal indices which take values in $s o(3)$ - the Lie algebra of $S O(3)$. Tildes are used to capture density weights of quantities; a tilde above indicates that the quantity transforms as a (tensor) density of weight 1 and a tilde below will denote a (tensor) density of weight -1 . The internal indices can be freely raised and lowered using a fixed kinematical metric $\dot{q}_{i j}$ on $s o(3)$. The phase space spanned by smooth pairs ( $\tilde{E}_{i}^{a}, K_{a}^{i}$ ) will be denoted by $\mathcal{P}$.

These phase space variables are related to their Arnowitt, Deser and Misner (ADM) [31] counterparts by

$$
\begin{align*}
& \tilde{E}_{i}^{a} \tilde{E}_{j}^{b} q^{i j}=\tilde{\tilde{q}} q^{a b}  \tag{2.2}\\
& K_{a}^{i} \tilde{E}_{i}^{b}=\widetilde{\sqrt{q}} K_{a}^{b} \tag{2.3}
\end{align*}
$$

where $q_{a b}$ is the metric on the leaf ${ }^{3} M, q$ its determinant, and $K_{a b}$ the extrinsic curvature of ${ }^{3} M$. In terms of these variables we perform a $3+1$ decomposition of space-time to obtain as Hamiltonian a sum of constraints with Lagrange multipliers [30, 32]:

$$
\begin{equation*}
H[\tilde{E}, K]=\int_{3_{M}}-\frac{1}{2} \underset{\sim}{N} \tilde{\tilde{S}}-\frac{1}{2} N^{a} \tilde{V}_{a}+\Lambda_{i} \tilde{G}^{i} \tag{2.4}
\end{equation*}
$$

The Lagrange multipliers $\underset{\sim}{N}, N^{a}$, the lapse and shift, are related to the choice of slicing and time in the standard fashion, and $\Lambda_{i}$ is related to rotations in the internal space. Phase space functions $\tilde{\tilde{S}}, \tilde{V}_{a}$, and $\tilde{G}^{k}$ are the scalar, vector, and Gauss constraints (with density weights $2,1,1$ respectively), given by $[30,32]$

$$
\begin{align*}
\tilde{\tilde{S}}(\tilde{E}, K) & \equiv-\tilde{\tilde{q}} \mathcal{R}-2 \tilde{E}_{[i}^{a} \tilde{E}_{j]}^{b} K_{a}^{i} K_{b}^{j}  \tag{2.5}\\
\tilde{V}_{a}(\tilde{E}, K) & \equiv 4 D_{[a}\left(K_{b]}^{i} \tilde{E}_{i}^{b}\right)  \tag{2.6}\\
\tilde{G}^{k}(\tilde{E}, K) & \equiv \epsilon_{i}^{j k} \tilde{E}_{j}^{a} K_{a}^{i} \tag{2.7}
\end{align*}
$$

Where $\mathcal{R}$ is the scalar curvature of the metric $q_{a b}$. The overall sign and numerical factors in the constraints are chosen so they reduce to the standard ADM constraints upon solving
the Gauss constraint. $\mathcal{R}$ can be written in terms of the triad and its inverse or in terms of the triad and the connection $\Gamma_{a}^{i}$ compatible with the triad, which is defined by

$$
\begin{equation*}
D_{a} \tilde{E}_{i}^{b}+\epsilon_{i j k} \Gamma_{a}^{j} \tilde{E}^{b k}=0, \quad \text { or } \quad \Gamma_{a}^{j}=-\frac{1}{2} \underset{\sim}{E} b k D_{a} \tilde{E}_{i}^{b} \epsilon^{i j k} \tag{2.8}
\end{equation*}
$$

(Note that $D_{a}$ acts only on tensor indices; it treats the internal indices as scalars.) Although $\Gamma_{a}^{i}$ is determined entirely by $\tilde{E}_{i}^{a}$ for now it is convenient to use all three fields $\Gamma_{a}^{i}, K_{a}^{i}$ and $\tilde{E}_{i}^{a}$ in our classical analysis: In our formulation of the BKL conjecture $\Gamma_{a}^{i}$ and $K_{a}^{i}$ will be the relevant degrees of freedom near the singularity, so it is natural to express the theory in terms of them.

The equations of motion are obtained by taking Poisson brackets with the Hamiltonian on the phase space $\mathcal{P}$ :

$$
\begin{align*}
\dot{\tilde{E}}_{i}^{a} & =\left\{\tilde{E}_{i}^{a}, H[\tilde{E}, K]\right\}  \tag{2.9}\\
\dot{K}_{a}^{i} & =\left\{K_{a}^{i}, H[\tilde{E}, K]\right\} \tag{2.10}
\end{align*}
$$

$\mathcal{P}$ is the phase space underlying LQG. The basic variables $\left(A_{a}^{i}, E_{i}^{a}\right)$ used there are obtained by a simple canonical transformation on $\mathcal{P}$ [30]:

$$
\begin{equation*}
\left(\tilde{E}_{i}^{a}, K_{a}^{i}\right) \rightarrow\left(A_{a}^{i}, \gamma^{-1} \tilde{E}_{a}^{i}\right) \quad \text { with } \quad A_{a}^{i}=\Gamma_{a}^{i}+\gamma K_{a}^{i} \tag{2.11}
\end{equation*}
$$

$\gamma$ being the Barbero-Immirzi parameter of LQC. (In classical general relativity, space-time equations of motion are independent of the value of this real parameter.) For simplicity of presentation we will introduce our formulation of the BKL conjecture using ( $\tilde{E}_{i}^{a}, K_{a}^{i}$ ) although it will be clear that our framework can be readily recast in terms of ( $\tilde{E}_{i}^{a}, A_{a}^{i}$ ).

## III. VARIABLES MOTIVATED BY THE BKL CONJECTURE

In order to formulate the BKL conjecture in this system, one needs to specify two things: What kind of derivatives are to dominate as one approaches the singularity and what kind are to become negligible? And, what are the quantities whose derivatives are to be treated as negligible? In this section we first motivate and introduce a set of variables and a derivative operator and then use them to formulate the conjecture. The main idea is as follows. The accumulated evidence to date suggests that the spatial metric $q_{a b}$ becomes degenerate at the space-like singularity whence its determinant $q$ vanishes there. (In particular, this is
borne out in the numerical simulations of solutions with two commuting Killing fields - the so-called $G 2$ space-times which include Gowdy models [33].) We will focus on the class of singularities where this occurs. In this case one would expect that if we rescaled fields which are ordinarily divergent at the singularity with appropriate powers of $q$, the rescaled quantities would have well defined limits.

Now, the density weighted triad $\tilde{E}_{i}^{a}$ is obtained by rescaling of the orthonormal triad $e_{i}^{a}$, which is divergent at the singularity, by $\sqrt{q}$. In examples, the factor of $\sqrt{q}$ not only gives $\tilde{E}_{i}^{a}$ a well defined limit, but the limit in fact vanishes. Therefore, contraction by $\tilde{E}_{i}^{a}$ can serve to tame fields which would otherwise have been divergent at the singularity. This consideration leads us to construct scalar densities by contracting $\tilde{E}_{i}^{a}$ with $K_{a}^{i}$, and $\Gamma_{a}^{i}$. As noted above, since contraction with $\tilde{E}_{i}^{a}$ will suppresses the divergence of $K_{a}^{i}$ and $\Gamma_{a}^{i}$, the combination is expected to remain finite at the singularity. Let us then set

$$
\begin{align*}
\tilde{P}_{i}{ }^{\prime} & :=\tilde{E}_{i}^{a} K_{a}^{j}-\tilde{E}_{k}^{a} K_{a}^{k} \delta_{i}{ }^{j}  \tag{3.1}\\
\tilde{C}_{i}^{j} & :=\tilde{E}_{i}^{a} \Gamma_{a}^{j}-\tilde{E}_{k}^{a} \Gamma_{a}^{k} \delta_{i}{ }^{j} . \tag{3.2}
\end{align*}
$$

These two fields, $\tilde{P}_{i}{ }^{j}$ and $\tilde{C}_{i}{ }^{j}$ will turn out to be the relevant variables near the singularity in our BKL framework. In particular, we will show below that the constraints of general relativity can be expressed in terms of polynomials of these basic variables and their derivatives. Therefore if the basic variables and their derivatives remain finite at the singularity, the constraints will also continue to hold there. Since the Hamiltonian of the theory is a linear combination of these constraints, dynamics of the basic variables will meaningfully extend to the singularity.

Beyond the possibility of being bounded at the singularity, an important feature of these variables is that they have only internal indices which can be freely raised and lowered using the fixed, kinematic, internal metric $\dot{q}^{i j}$; the dynamical metric $q^{a b}$ which diverges at singularities is not needed. Under diffeomorphisms $\tilde{P}_{i}{ }^{j}$ and $\tilde{C}_{i}{ }^{j}$ transform as density weighted scalars on ${ }^{3} M$. Because of this feature, statements about their asymptotic properties can be formulated much more easily than would be possible if they were tensor fields. (For a coordinate free introduction to densities, see Appendix A).

To illustrate why these variables are likely to be well defined at the singularity, let us consider the Bianchi I model. Because of spatial flatness, we can work in an internal gauge in which $C_{i}{ }^{j}=0$ everywhere. What about $\tilde{E}_{i}^{a}$ and $P_{i}{ }^{j}$ ? In terms of the commonly used
proper time $\tau$, the metric is given by $d s^{2}=-d \tau^{2}+\sum_{i} \tau^{2 p_{i}} d x_{i}^{2}$ and the singularity occurs at $\tau=0$. Since $\sum p_{i}=1$, we have $q=\tau^{2}$ in the Bianchi I chart. In addition, due to the second constraint on the exponents, $\sum p_{i}^{2}=1$ whence the density weighted triad $\tilde{E}_{i}^{a}$ vanishes at the singularity as $\tau^{1-p_{i}}$ and $P_{i}^{j}$ is finite there for each $i$.

We further introduce a derivative operator $\tilde{D}_{i}$ defined by the contraction of $D_{a}$ with $\tilde{E}_{i}^{a}$ :

$$
\begin{equation*}
\tilde{D}_{i}:=\tilde{E}_{i}^{a} D_{a} \tag{3.3}
\end{equation*}
$$

The expectation is that this contraction will have the effect of suppressing terms containing $\tilde{D}_{i}$ as we approach the singularity. Thus, $\tilde{D}_{i}$ will be the spatial derivatives we were seeking which, when acting on certain quantities, will be conjectured to be negligible near the singularity. ${ }^{2}$ The variable $\tilde{P}_{i j}$ is related to the momentum $\tilde{P}^{a b}$ (conjugate to the 3-metric) in the ADM phase space by $\tilde{\tilde{q}} \tilde{P}^{a b}=\tilde{E}_{i}^{a} \tilde{E}_{j}^{b} \tilde{P}^{i j} . \tilde{C}_{i j}$ encodes information in the $\tilde{D}_{i}$ spatial derivatives of the triad $\tilde{E}_{i}^{a}$ :

$$
\begin{equation*}
\tilde{C}^{i j}=-\underset{\sim}{E_{a}^{i}} \epsilon^{k l j} \tilde{D}_{k} \tilde{E}_{l}^{a} . \tag{3.4}
\end{equation*}
$$

Note that, although the $\tilde{C}_{i j}$ depend on spatial derivatives of the triad and are often subdominant to $\tilde{P}_{i j}$, it turns out that they are not always negligible in the approach to the singularity. Indeed, this behavior is observed in the truncated system, which is discussed in section IV. It is $\tilde{C}^{i j}$ rather than the triads themselves that will feature directly in our formulation of the conjecture.

For simplicity of notation, from now on we will drop the tildes. Thus, from now on each of $E_{i}^{a}, C_{i}{ }^{j}, P_{i}^{j}, D_{i}$ carries a density weight 1 , while the lapse field $N$ carries a density weight -1 . The scalar and the vector constraint functions $S$ and $V_{i}$ (introduce below) carry density weight 2 while the Gauss constraint $G^{k}$ carries density weight 1.

By making use of (3.1) and (3.4), functions of $\left(E_{i}^{a}, K_{a}^{i}\right)$ and their covariant derivatives can be rewritten in terms of $\left(E_{i}^{a}, C_{i}{ }^{j}, P_{i}{ }^{j}\right)$ and their $D_{i}$ derivatives. The scalar curvature $\mathcal{R}$ for example can be expressed entirely in terms of $C_{i}{ }^{j}$ and its $D_{i}$ derivatives:

$$
\begin{equation*}
q \mathcal{R}=-2 \epsilon^{i j k} D_{i}\left(C_{j k}\right)-4 C_{[i j]} C^{[i j]}-C_{i j} C^{j i}+\frac{1}{2} C^{2} \tag{3.5}
\end{equation*}
$$

[^2]Consequently, the constraints can be re-expressed entirely in terms of $C_{i}{ }^{j}, P_{i}{ }^{j}$ and their $D_{i}$ derivatives (with no direct reference to $E_{i}^{a}$ or even the determinant $q$ of the 3-metric):

$$
\begin{align*}
S & =2 \epsilon^{i j k} D_{i}\left(C_{j k}\right)+4 C_{[i j]} C^{[i j]}+C_{i j} C^{j i}-\frac{1}{2} C^{2}+P_{i j} P^{j i}-\frac{1}{2} P^{2}  \tag{3.6}\\
V_{i} & =-2 D_{j} P_{i}^{j}-2 \epsilon_{j k l} P_{i}^{j} C^{k l}-\epsilon_{i j k} C P^{j k}+2 \epsilon_{i j k} P^{j l} C_{l}^{k}  \tag{3.7}\\
G^{k} & =\epsilon^{i j k} P_{j i} . \tag{3.8}
\end{align*}
$$

Here we have converted the co-vector index on the vector constraint $V_{a}$ to an internal index by contracting it with $E_{i}^{a}$. Since the $E_{i}^{a}$ is assumed to be non-degenerate away from the singularity the constraint $V_{i}$ defines the same constraint surface as the original vector constraint introduced in (2.5). Notice here that the constraint can be easily decomposed into those terms that contain the derivative $D_{i}$ and those that don't.

The equations of motion for $E_{i}^{a}, C_{i}{ }^{j}, P_{i}{ }^{j}$ can be written in a similar form. These can be obtained using the full Poisson brackets (2.9),(2.10) or by directly computing Poisson brackets of $P_{i}{ }^{j}$ and $C_{i}{ }^{j}$ with the scalar/Hamiltonian constraint. To streamline the second calculation, let us specify the Poisson brackets between $E_{i}^{a}, C_{i}{ }^{j}$, and $P_{i}{ }^{j}$ :

$$
\begin{align*}
\left\{E_{i}^{a}(x), P_{j}^{k}(y)\right\} & =\left(E_{j}^{a}(x) \delta_{i}^{k}-E_{i}^{a}(x) \delta_{j}^{k}\right) \delta(x, y)  \tag{3.9}\\
\left\{P_{i}^{j}(x), P_{k}{ }^{l}(y)\right\} & =\left(P_{k}{ }^{j}(x) \delta_{i}^{l}-P_{i}^{l}(x) \delta_{k}^{j}\right) \delta(x, y)  \tag{3.10}\\
\left\{\int f_{i j} P^{i j}, \int g_{k l} C^{k l}\right\} & =\int\left(f_{i j} g_{k l}\left(C^{k j} \delta^{i l}+C^{j l} \delta^{i k}\right)+\epsilon^{j l m} \delta^{i k} g_{k l} D_{m} f_{i j}\right)  \tag{3.11}\\
\left\{E_{i}^{a}(x), C^{j}{ }_{k}(y)\right\} & =0 \quad \text { and } \quad\left\{C_{i}^{j}(x), C_{k}^{l}(y)\right\}=0, \tag{3.12}
\end{align*}
$$

where $f_{i j}, g_{i j}$ are smooth test scalar fields. The equations of motion obtained by taking Poisson brackets with the scalar constraint are then given by

$$
\begin{align*}
\dot{C}^{i j}=- & \epsilon^{j k l} D_{k}\left(N\left(\frac{1}{2} \delta_{l}^{i} P-P_{l}{ }^{i}\right)\right)+N\left[2 C_{k}^{(i} P^{|k| j)}+2 C^{[k j]} P_{k}^{i}-P C^{i j}\right]  \tag{3.13}\\
\dot{P}^{i j}= & \epsilon^{j k l} D_{k}\left(N\left(1 / 2 \delta_{l}^{i} C-C_{l}^{i}\right)\right)-\epsilon^{k l m} D_{m}\left(N C_{k l}\right) \delta^{i j}+2 \epsilon^{j k m} C^{[i k]} D_{m}(N) \\
& \left(D^{i} D^{j}-D^{k} D_{k} \delta^{i j}\right) N+N\left[-2 C^{(i k)} C_{k}^{j}+C C^{i j}-2 C^{[k l]} C_{[k l]} \delta^{i j}\right] \tag{3.14}
\end{align*}
$$

and

$$
\dot{E}_{i}^{a}=-N P_{i}{ }^{j} E_{j}^{a}
$$

where we have set the shift to zero to reduce clutter. (For non-zero shift, see Appendix B.) Note that the equation of motion for $E_{i}^{a}$ is a simple ODE. Note also that, as was the case with constraints, the equations of motion for $C_{i}{ }^{j}$ and $P_{i}{ }^{j}$ can again be written in terms
of scalar densities and the derivative $D_{i}$ only. This motivates us to ask for an evolution equation for the derivative operator $D_{i}$. Since $D_{i}$ ignores internal indices, it suffices to consider its action just on scalar densities $S_{n}$ of weight $n$. We have:

$$
\begin{equation*}
\dot{D}_{i} S_{n}=\frac{n}{2}\left[D_{i}(N P)\right] S_{n}-N P_{i}^{j} D_{j} S_{n} \tag{3.15}
\end{equation*}
$$

Thus we have cast all the constraint as well as evolution equations as a closed system involving only $C_{i}{ }^{j}, P_{i}{ }^{j}$, and $D_{i}$. These equations can then be used as follows. On an initial slice, we construct $\left(C_{i}^{j}, P_{i}^{j}, D_{i}\right)$ from a pair $\left(E_{i}^{a}, K_{a}^{i}\right)$ of canonical variables. Then we can deal exclusively with the triplet $\left(C_{i}^{j}, P_{i}^{j}, D_{i}\right)$. The pair $\left(E_{i}^{a}, K_{a}^{i}\right)$ satisfies constraints if and only if the triplet satisfies (3.6)-(3.8). Given such a triplet, we can evolve it using (3.13),(3.14),(3.15) without having to refer back to the original canonical pair $\left(E_{i}^{a}, K_{a}^{i}\right)$. These two sets of equations have some interesting unforeseen features. First, as already mentioned, the basic triplet $\left(C_{i}{ }^{j}, P_{i}{ }^{j}, D_{i}\right)$ has only internal indices: our basic fields are scalars on ${ }^{3} M$ (with density weight 1 ). It would be of considerable interest to investigate if this fact provides new insights into the dynamics of $3+1$ dimensional gravity [35]. Second, these equations do not refer to the triad $E_{i}^{a}$. Suppose we begin at an initial time where $C_{i}{ }^{j}$ is derived from an $E_{i}^{a}$. Then these constraint and evolution equations ensure that $C_{i}{ }^{j}$ is derivable from a triad at all times. Furthermore, we can easily construct that triad directly from a solution $\left(C_{i}{ }^{j}, P_{i}{ }^{j}\right)$ to these equations: first solve (3.13)-(3.15) and then simply integrate the ODE

$$
\begin{equation*}
\dot{E}_{i}^{a}=-N P_{i}^{j} E_{j}^{a} \tag{3.16}
\end{equation*}
$$

at the end. Third, the structure of the constraint and evolution equations in terms of $\left(C_{i}{ }^{j}, P_{i}{ }^{j}, D_{i}\right)$ is remarkably simple since only low order polynomials of these variables are involved. Finally, thanks to our rescaling by $\sqrt{q}$, our basic triplet $C_{i}{ }^{j}, P_{i}{ }^{j}, D_{i}$ (as well as $\left.E_{i}^{a}\right)$ are expected to have a well behaved limit at the singularity. A close examination of our equations shows that they allow the triad become to become degenerate during evolution. So, strictly (as in LQG [30, 32]) we have a generalization of Einstein's equations.

To summarize, we have found variables which remain finite at the singularity in examples and rewritten Einstein's equations as a closed system of differential equations in terms of them. Therefore, this formulation may be useful for proving global existence and uniqueness results and rigorous exploration of fields near space-like singularities. Finally, although for
simplicity we have set shift $N^{i}$ and the smearing field $\Lambda_{i}$ equal to zero, the features we just discussed hold more generally (see Appendix B).

To conclude, let us examine the action of the vector and the Gauss constraints on our basic variables. (The action of the scalar constraint yields the evolution equations which we have already discussed.) Since the vector constraint generates a combination of spatial diffeomorphisms and internal rotations, it is standard to subtract a multiple of the Gauss constraint to define the diffeomorphism constraint:

$$
\begin{equation*}
V_{i}^{\prime}=V_{i}-2\left(C_{i}^{j}-\frac{C}{2} \delta_{i}^{j}\right) G_{j} \tag{3.17}
\end{equation*}
$$

We can then smear both constraints to obtain

$$
\begin{equation*}
G[\Lambda]=\int_{{ }_{3} M} \Lambda^{k} G_{k} \quad \text { and } \quad V^{\prime}[N]=\int_{3_{M}} N^{i} V_{i}^{\prime} \tag{3.18}
\end{equation*}
$$

where $N^{i} \mathrm{~s}$ a scalar with density weight -1 so that $N^{a}:=N^{i} E_{i}^{a}$ is the standard lapse and, as before, $\Lambda^{i}$ has density weight zero. The action of $G[\Lambda]$ on the basic variables is given as usual via Poisson brackets:

$$
\begin{align*}
\left\{P_{i j}, G[\Lambda]\right\} & =\epsilon_{k l j} \Lambda^{l} P_{i}^{k}+\epsilon_{k l i} \Lambda^{l} P_{j}^{k}  \tag{3.19}\\
\left\{C_{i j}, G[\Lambda]\right\} & =\epsilon_{k l j} \Lambda^{l} C_{i}^{k}+\epsilon_{k l i} \Lambda^{l} C_{j}^{k}+D_{i} \Lambda_{j}-D_{k} \Lambda^{k} \delta_{i j}  \tag{3.20}\\
\left\{D_{i} S_{n}, G[\Lambda]\right\} & =\epsilon_{j k i} \Lambda^{k} D^{j} S_{n} \tag{3.21}
\end{align*}
$$

In the last equation $S_{n}$ is any scalar density of weight n . As expected the Gauss constraint generates infinitesimal $S O(3)$ transformations with $D_{i} S_{n}$ and $P_{i}{ }^{j}$ transforming as tensors and $C_{i}{ }^{j}$ transforming as (the contraction of a triad with) an $S O(3)$ connection.

Similarly, the action of the diffeomorphism constraint is given by the Poisson brackets:

$$
\begin{align*}
\left\{P_{i}{ }^{j}, V^{\prime}[N]\right\} & =-2\left(N^{k} D_{k} P_{i}{ }^{j}+P_{i}{ }^{j} D_{k} N^{k}+P_{i}{ }^{j} \epsilon_{k l m} N^{k} C^{l m}\right)=-2 \mathcal{L}_{\vec{N}} P_{i}^{j}  \tag{3.22}\\
\left\{C_{i}^{j}, V^{\prime}[N]\right\} & =-2\left(N^{k} D_{k} C_{i}^{j}+C_{i}^{j} D_{k} N^{k}+C_{i}^{j} \epsilon_{k l m} N^{k} C^{l m}\right)=-2 \mathcal{L}_{\vec{N}} C_{i}^{j}  \tag{3.23}\\
\left\{D_{i} S_{n}, V^{\prime}[N]\right\} & =-2\left(N^{j} D_{j}\left(D_{i} s_{n}\right)+n D_{j}\left(N^{j}\right) D_{i} S_{n}-n \epsilon_{j k l} N^{j} C^{k l} D_{i} S_{n}\right)=-2 \mathcal{L}_{\vec{N}} D_{i} S_{n} \tag{3.24}
\end{align*}
$$

where $\vec{N} \equiv N^{a}=E_{i}^{a} N_{i}$. We see that the constraint generates diffeomorphisms as expected with $P_{i}{ }^{j}, C_{i}{ }^{j}$, and $D_{i} S_{n}$ transforming as scalar densities. Again, note that the infinitesimal changes generated by each constraint involve only the basic variables $C_{i}{ }^{j}, P_{i}{ }^{j}$, and $D_{i}$. Thus there is still a closed system in terms of this set of variables.

## IV. THE CONJECTURE

In order to express the BKL conjecture we must make more precise the arena in which it is to be applied. The ingredients we need are a space-time with a space-like singularity, a notion of 'spatial' and 'temporal' derivatives, and specification of the system to which the conjecture is to be applied. We make use of the framework introduced in the previous section to provide this arena.

Let us begin with a 4 -manifold, ${ }^{4} M$ admitting a smooth foliation $M_{t}$ parameterized by a time function, $t$. We restrict ourselves to a slicing of ${ }^{4} M$ in which the space-like singularity lies on the limiting leaf. This ensures that we can reasonably discuss an approach to the singularity as approaching the limiting leaf. The time function $t$ labeling our spatial slices is intertwined with the choice of lapse and shift. We will assume that the lapse $N$ and the shift $N^{i}$, each with density weight -1 , admit a smooth limit as one approaches the singularity. Since the spatial metric $q_{a b}(t)$ becomes degenerate at the singularity, the commonly used lapse function $\bar{N}:=\sqrt{q} N$ (with density weight zero) goes to zero, thus placing the singularity at $t=\infty$. (These assumptions are minimal and further constraints on admissible foliations may well be needed in a more complete framework.)

Our basic variables will be $\left(C_{i}{ }^{j}, P_{i}^{j}\right)$, the lapse $N$, and the shift $N^{i}$. By time derivatives, we will mean their Lie derivatives along the vector field $t^{a}:=\bar{N} n^{a}+N^{a}$ where $n^{a}$ is the unit normal to the foliation $M_{t}$. By spatial derivatives we will mean their $D_{i}$ derivatives. Since $D_{i}:=E_{i}^{a} D_{a}$, the notion does not depend on coordinates. Rather, it is tied directly to the physical triads and the covariant derivatives compatible with them. Then, the idea behind the conjecture is that, as one approaches the singularity, the spatial derivatives $D_{i} C_{j}{ }^{k}, D_{i} P_{j}{ }^{k}, D_{i} N, D_{i} N^{j}$ of the basic fields should become negligible compared to the basic fields themselves because of the $\sqrt{q}$ multiplier in the definition of $E_{i}^{a}$ which descends to $D_{i}$.

We now show that an immediate consequence of this assumption is that the antisymmetric part of $C_{i j}$ is negligible compared to the other basic fields. Let us define $a^{i}:=\epsilon^{i j k} C_{j k}$. Then by conjecture $D_{i}\left(a^{i} N\right)$ is negligible. ${ }^{3}$ Since the spatial manifold is assumed to be compact,

[^3]integrating this negligible quantity and then integrating by parts, one obtains:
\[

$$
\begin{equation*}
\int_{{ }_{3} M} D_{i}\left(N a^{i}\right)=\int_{{ }_{3} M} N a^{i} D_{a} E_{i}^{a}=\int_{{ }_{3} M} N a^{i} a_{i} \tag{4.1}
\end{equation*}
$$

\]

where we have used the definition of $C_{i j}$ which implies $D_{a} E_{i}^{a}=\epsilon_{i j k} C^{j k}$. Since the internal metric and the lapse are positive, we conclude that $a_{i}$ and hence $C_{[i j]}$ are necessarily negligible under our assumptions. This fact will be useful throughout our analysis.

Next, note that we have expressed general relativity in the form of a constrained theory in terms of our basic variables, $C_{i}{ }^{j}, P_{i}{ }^{j}$, and $D_{i}$. Our constraints are composed of quadratic terms in our basic variables and terms of the form $D_{i} C_{j}{ }^{k}$ and $D_{i} P_{j}{ }^{k}$. We can therefore split each constraint into two parts - terms which contain no derivatives and those which do. Similarly the equations of motion can be split into terms that contain derivatives and those that do not. With this background, we can state two versions of our conjecture.

Weak Conjecture : As the singularity is approached the terms containing derivatives in the constraints and equations of motion are negligible in comparison to the polynomial terms. Thus, as the singularity is approached the constraints and equations of motion approach those found by setting derivative terms to zero.

We define the truncated theory to be the system defined by setting $D_{i}$-derivative terms to zero,

$$
\begin{equation*}
D_{i} C_{j}^{k}=D_{i} P_{j}^{k}=D_{i} N=D_{i} N_{j}=C_{[i j]}=0 \tag{4.2}
\end{equation*}
$$

in the equations of motion (3.13)-(3.15) and constraints (3.6)-(3.8). Thus, the weak conjecture says that the equations of motion can be well approximated by those of the truncated theory in the vicinity of the singularity. Note that this does not imply that the solutions of the full equations of motion will approach the solutions to the truncated equations as the singularity is approached. This additional condition is captured in the strong version as follows.

Strong Conjecture: As the singularity is approached the constraints and the equations of motion approach those of the truncated theory and in addition the solutions to the full equations are well approximated by solutions to the truncated equations.

With the strong conjecture the solution of the full Einstein equations will asymptote to solutions of the truncated system defined by (4.2). In the following we will analyze this truncated system.

Not only are the truncated constraints purely algebraic, but they involve only quadratic combinations our basic variables:

$$
\begin{align*}
S_{(T)} & :=C_{i j} C^{j i}-\frac{1}{2} C^{2}+P_{i j} P^{j i}-\frac{1}{2} P^{2}  \tag{4.3}\\
V_{i}^{(T)} & :=-\epsilon_{i j k} C P^{j k}+2 \epsilon_{i j k} P^{j l} C_{l}^{k}  \tag{4.4}\\
G_{(T)}^{k} & :=\epsilon^{i j k} P_{j i}, \tag{4.5}
\end{align*}
$$

The truncated Gauss constraint is in fact exact because (3.8) involves no derivative terms, while the scalar and the diffeomorphism constraints are genuinely truncated.

The infinitesimal transformations (3.19) - (3.24) generated by the full constraints contain derivative terms that are now assumed to be negligible in comparison to the polynomial terms. Ignoring the negligible terms leads us to the following transformations on the basic fields:

$$
\begin{align*}
\left\{P_{i j}, G(\Lambda)\right\}_{T} & =2 \epsilon_{k l(j} P_{i)}{ }^{k} \Lambda^{l}  \tag{4.6}\\
\left\{C_{k l}, G(\Lambda)\right\}_{T} & =2 \epsilon_{k l(j} C_{i)}{ }^{k} \Lambda^{l}  \tag{4.7}\\
\left\{P_{i j}, V(N)\right\}_{T} & =4 \epsilon_{k l(j} P_{i}{ }^{k} N^{m}\left(C_{m}^{l}-\frac{C}{2} \delta_{m}^{l}\right)  \tag{4.8}\\
\left\{C_{i j}, V(N)\right\}_{T} & =4 \epsilon_{k l(j} C_{i)}^{k} N^{m}\left(C_{m}^{l}-\frac{C}{2} \delta_{m}^{l}\right)  \tag{4.9}\\
\left\{C_{i j}, S(N)\right\}_{T} & =-2 N\left(2 C_{k(i} P_{j)}^{k}-P C_{i j}\right)  \tag{4.10}\\
\left\{P_{i j}, S(N)\right\}_{T} & =-2 N\left(-2 C_{i k} C_{j}^{k}+C C_{i j}\right) \tag{4.11}
\end{align*}
$$

The Gauss constraint continues to generate internal rotations, but, whereas in the full theory $C_{i}{ }^{j}$ transforms as (the contraction of the triad with) a connection, after truncation both $C_{i}{ }^{j}$ and $P_{i}{ }^{j}$ transform as $S O(3)$ tensors. The vector constraint also generates internal rotations, since the diffeomorphism constraint generates only negligible terms.

We arrived at the truncated equations of motion by first obtaining the full equations and then applying the truncation to them i.e., by setting spatial derivative terms to zero. But we could also have first truncated the constraints to obtain (4.3)- (4.5) and then computed their truncated Poisson brackets with the basic variables. This leads to a consistency check of our scheme: do the two procedure yield the same 'truncated equations of motion' in the end?

The answer is in the affirmative. This fact is illustrated by the following 'commutativity diagram':

Full Constraint $\xrightarrow{\text { Truncation }}$ Truncated Constraint


Full Equation of Motion $\xrightarrow{\text { Truncation }}$ Truncated Equation of Motion
Note that the operation of truncation, the final truncated system, and hence the consistency requirement mentioned above depends crucially on one's choice of basic variables and notions of space and time derivatives. For example, if we had adopted the more 'obvious' strategy and used triads $E_{i}^{a}$ rather than $C_{i}{ }^{j}$ as basic variables, we would have been led to set $C_{i}{ }^{j}$ to zero in the truncation procedure since $C_{i}{ }^{j}$ would then be derived quantities, obtained by taking the $D_{i}$ derivative of $E_{i}^{a}$. This truncation would have led us just to Bianchi I equations. The resulting BKL conjecture would have been manifestly false. Thus, considerable care is needed to arrive at variables which satisfy a closed set of equations in a Hamiltonian framework, suggest a natural way to make the heuristic idea of ignoring spatial derivatives in favor of time derivatives precise, lead to the above commuting diagram, and a version of the BKL conjecture that is compatible with the large body of analytical and numerical results that has accumulated so far. It is rather striking that the variables $\left(C_{i}{ }^{j}, P_{i}{ }^{j}\right)$ automatically satisfy these rather stringent criteria.

## V. HAMILTONIAN FORMULATION OF THE TRUNCATED SYSTEM

In this section we will analyze the truncated system in some detail and show that its solutions reproduce the expected BKL behavior. The section is divided into three parts. In the first we regard $C_{i}{ }^{j}, P_{i}{ }^{j}$ as fields on the full phase space $\mathcal{P}$, obtain the truncated Poisson brackets between them and truncated constraints. In the second we solve and gauge fix the vector and the Gauss constraints of the truncated theory. The result is a finite dimensional, reduced phase space with a single constraint which is well suited to serve as a starting point for quantization inspired by the BKL conjecture. In the third part we discuss several features of solutions to this Hamiltonian theory. In particular, we will find that they exhibit Bianchi I phases with Bianchi II transitions.

## A. Truncated Poisson brackets

Since the truncated equations of motion can be formulated entirely in terms of $C_{i}{ }^{j}, P_{i}{ }^{j}$, let us truncate the Poisson brackets (3.10), (3.11) we obtained between them by setting the negligible terms on the right side to zero. Since the full Poisson bracket (3.11) involves smearing fields $f_{i j}$ and $g_{i j}$ we first need to specify which terms involving them are to be regarded as negligible. The most natural avenue is to construct to $f_{i j}$ and $g_{i j}$ only from the basic fields $\left(C_{i}{ }^{j}, P_{i}{ }^{j}, N, N_{i}, \stackrel{q}{q}_{i j}, \epsilon^{i j k}\right)$ (and their $D_{i}$ derivatives). Then the terms containing $D_{i}$ derivatives of the smearing fields will also be negligible and hence vanish in the truncation. The resulting truncated Poisson brackets between $C_{i}{ }^{j}$ and $P_{i}{ }^{j}$ are then given by:

$$
\begin{align*}
\left\{P_{i}^{j}(x), C_{k}^{l}(y)\right\}_{T} & =\left(C_{k}^{j} \delta_{i}^{l}+C^{j l} \delta_{i k}\right)(x) \delta(x, y)  \tag{5.1}\\
\left\{P_{i}^{j}(x), P_{k}^{l}(y)\right\}_{T} & =\left(P_{k}^{j} \delta_{i}^{l}-P_{i}^{l} \delta_{k}^{j}\right)(x) \delta(x, y)  \tag{5.2}\\
\left\{C_{i}^{j}(x), C_{k}^{l}(y)\right\}_{T} & =0 \tag{5.3}
\end{align*}
$$

These Poisson brackets suffice to determine the equations of motion because the truncated Hamiltonian constraint (4.3) is algebraic in $C_{i}{ }^{j}$ and $P_{i}{ }^{j}$. They are now ODEs,

$$
\begin{equation*}
\dot{C}_{i j}=N\left[2 C_{k(i} P_{j)}^{k}-P C_{i j}\right] \quad \text { and } \quad \dot{P}_{i j}=N\left[-2 C_{i k} C^{k}{ }_{j}+C C_{i j}\right], \tag{5.4}
\end{equation*}
$$

so the truncated dynamics at any one spatial point decouple from those at other points.
This system has some notable features. First, we have a closed system expressed entirely in terms of $C_{i}{ }^{j}(x)$ and $P_{i}{ }^{j}(x)$ at any fixed point $x$. Furthermore, the equations of motion (5.4) and constraints (4.3)-(4.5) are at most quadratic in these variables. In the full theory, the triad does not appear explicitly in the equations (3.13) - (3.15) but is implicitly present through $D_{i}$. Upon truncation, even this implicit dependence disappears. Second, as in the full theory, one can first solve the equations of motion for $C_{i}{ }^{j}(x)$ and $P_{i}{ }^{j}(x)$ and then evolve the triad at that point at the end by solving an ODE. Third, the truncated scalar constraint (4.3) is symmetric under interchange of $C_{i}{ }^{j}$ and $P_{i}{ }^{j}$ and, by adding a multiple of the Gauss constraint, the vector constraint can be made anti-symmetric under this interchange:

$$
\begin{equation*}
\bar{V}_{(T)}^{i}:=\epsilon^{i j k} P_{j}^{l} C_{k l} \tag{5.5}
\end{equation*}
$$

However, this symmetry is broken at the level of equations of motion because the truncated Poisson algebra does not have a simple transformation property under this interchange.

Because fields at distinct points decouple, to study the truncated system from the viewpoint of differential equations, one can simply restrict oneself to a single spatial point. However, this is not directly possible in the Hamiltonian framework because even in the truncated theory, the Poisson brackets (5.1), (5.2) involve $\delta(x, y)$. But one can introduce a subspace $\mathcal{P}_{\text {hom }}$ of the full phase space $\mathcal{P}$ tailored to our truncation. Given a point $\left(E_{i}^{a}, K_{a}^{i}\right)$ in $\mathcal{P}$ consider the pair $\left(C_{i}{ }^{j}, P_{i}{ }^{j}\right)$ of density weighted fields it determines. The phase space point will be said to be homogeneous if there exists an internal gauge and a nowhere vanishing scalar density $S_{-1}$ of weight -1 such that the (density weight zero) scalar fields $\left(S_{-1} C_{i}^{j}, S_{-1} P_{i}^{j}\right)$ are constants on ${ }^{3} M$ (and $C_{[i j]}=0$ ). (Fixing a $S_{1}$ is equivalent to fixing a 3-form on ${ }^{3} M$; see Appendix A.) Clearly, the truncated dynamics leaves this homogeneous sub-space $\mathcal{P}_{\text {hom }}$ of the phase space invariant. More importantly, $\mathcal{P}_{\text {hom }}$ is invariant under full dynamics: If the $D_{i}$-derivatives are initially zero they remain zero under the full equations of motion. The Hamiltonian dynamics on $\mathcal{P}_{\text {hom }}$ fully captures the truncated dynamics at any fixed spatial point on ${ }^{3} M$.

Remark: Since the triads $E_{i}^{a}$ in the full phase space $\mathcal{P}$ have been assumed to be nondegenerate, they are also non-degenerate in $\mathcal{P}_{\text {hom }}$. However, as examples suggest, one would expect them to be become degenerate in the limit to the space-like singularity where, however, $C_{i}{ }^{j}, P_{i}{ }^{j}$ would continue to be well behaved (and some of them may even vanish). It is therefore of some interest to extend the homogeneous subspace by adding 'limit points' which have this behavior. This construction is not needed in our analysis. However, since it may be useful in future investigations, we will conclude this subsection with a brief summary. Let us allow the density weighted triads $E_{i}^{a}$ to become degenerate such that the subspaces spanned by the non-degenerate directions of vector fields $S_{-1} E_{i}^{a}$ are integrable. (If this condition is satisfied for one nowhere vanishing scalar density $S_{-1}$, it is satisfied for all.) Thus, in the degenerate case we obtain preferred 2 or 1 dimensional sub-manifolds on ${ }^{3} M$. We can extend the phase space by including such degenerate $E_{i}^{a}$ if, in addition, the resulting pair $\left(C_{i}^{j}, P_{i}^{j}\right)$ is regular, $C_{i j}$ is symmetric and the pair $S_{-1} C_{i}^{j}, S_{-1} P_{i}{ }^{j}$ is homogeneous along the preferred lower dimensional sub-manifolds of ${ }^{3} M$. Key questions for the BKL conjecture are then: i) Does the Hamiltonian flow on $\mathcal{P}$ naturally extend to this extension?; and ii) Do generic dynamical trajectories flow to it?

## B. Reduced Phase Space

Since $C_{i j}$ is symmetric but $P_{i j}$ is not, the homogeneous subspace $\mathcal{P}_{\text {hom }}$ is not a symplectic sub-manifold of the full phase space $\mathcal{P}$. But it turns out that one can obtain a symplectic manifold by solving and gauge fixing the truncated vector and the Gauss constraints. It will be referred to as the reduced phase space, $\mathcal{P}_{\text {red }}$.

The Gauss constraint (4.5) is equivalent to asking that $P_{i j}$ is symmetric and then the vector constraint (4.4) is equivalent to asking that as matrices, $C_{i}{ }^{j}$ and $P_{i}{ }^{j}$ should commute. To gauge fix the Gauss constraint, we first note the transformation properties (4.6) and (4.7) of $P_{i}^{j}$ and $C_{i}^{j}$ under the action of the Gauss constraint. It is easy to verify that, because $P_{i}{ }^{j}$ and $C_{i}{ }^{j}$ commute, the requirement that they both be diagonal gauge-fixes the Gauss constraint completely. It turns out that the diagonality requirement also fixes the vector constraint. This may seem surprising at first. But note that the combination $\bar{V}$ of the vector and the Gauss constraint of Eq (5.5) again generates internal gauge rotations, where, however the generator $\Lambda^{i}$ is a ' $q$-number', i.e., depends on the phase space variables: $\Lambda^{i}=N^{j}\left(C^{i}{ }_{j}-C \delta_{j}^{i}\right)$, where $N^{j}$ is the shift used to smear the vector constraint. The fact that the gauge fixing of the vector constraint does not impose additional requirements on ( $C_{i j}, P_{i j}$ ) 'cures' the mismatch in the degrees of freedom in the homogeneous subspace (arising from the fact that while $C_{i j}$ is symmetric, $P^{i j}$ is not.).

So far $C_{i}{ }^{j}, P_{i}^{j}$ are fields on ${ }^{3} M$, each carrying density weight 1 . Since these fields are homogeneous, symmetric and diagonal, the reduced phase space is 6 dimensional. It is convenient to coordinatize it with just six numbers, $C_{I}, P^{I}$, with $I=1,2,3$ :

$$
\begin{equation*}
C_{1}:=\int_{3_{M}} C_{1}^{1} ; \quad P^{1}:=\int_{3_{M}} P_{1}^{1} ; \quad \text { etc } \tag{5.6}
\end{equation*}
$$

where the integrals are well defined because we have completely fixed the internal gauge, in that gauge the integrands are all densities of weight 1 , and ${ }^{3} M$ is compact. From now on we will focus on the description of $\mathcal{P}_{\text {red }}$ in terms of $C_{I}$ and $P^{I}$.

The symplectic structure on $\mathcal{P}_{\text {red }}$ is given by the Poisson brackets: ${ }^{4}$

$$
\begin{equation*}
\left\{P^{I}, P^{J}\right\}=\left\{C_{I}, C_{J}\right\}=0 \quad \text { and } \quad\left\{P^{I}, C_{J}\right\}=2 \delta_{J}^{I} C_{J} \tag{5.7}
\end{equation*}
$$

[^4]The scalar or Hamiltonian constraint

$$
\begin{equation*}
\frac{1}{2} C^{2}-C_{I} C^{I}+\frac{1}{2} P^{2}-P_{I} P^{I}=0 \tag{5.8}
\end{equation*}
$$

now generates the equations of motion via Poisson brackets:

$$
\begin{array}{r}
\dot{P}_{I}=N C_{I}\left(C-2 C_{I}\right) \\
\dot{C}_{I}=-N C_{I}\left(P-2 P_{I}\right) \tag{5.10}
\end{array}
$$

Here and in what follows we use the summation convention also for the indices $I, J$ and have set

$$
\begin{equation*}
P=P_{1}+P_{2}+P_{3} \quad \text { and } \quad C=C_{1}+C_{2}+C_{3} \tag{5.11}
\end{equation*}
$$

As a side remark, we note that $C_{I}=0$ is a fixed point of our system for each $C_{I}$, whence the sign of each $C_{I}$ along any dynamical trajectory is fixed by the initial conditions. Therefore, away from the 'planes' $C_{I}=0$, we can, if we wish, perform a change of variables to $X_{I}=$ $\ln \left|C_{I}\right| / 2$ and work with the canonically conjugate pair $\left(X^{I}, P_{I}\right)$. However, in what follows, we will continue to work with $\left(C_{I}, P^{I}\right)$.

Finally, recall that in the BKL conjecture 'the only matter that matters' is a scalar field. Let us therefore extend our gravitational reduced phase space to include a massless scalar field $\phi$. Denote the conjugate momentum by $\pi$ so that $\{\phi, \pi\}=1$. Then on this extended reduced phase space $\overline{\mathcal{P}}_{\text {red }}$ the Hamiltonian constraint is given by

$$
\begin{equation*}
\frac{1}{2} C^{2}-C_{I} C^{I}+\frac{1}{2} P^{2}-P_{I} P^{I}-\frac{\pi^{2}}{2}=0 \tag{5.12}
\end{equation*}
$$

The equations for $\dot{P}$ and $\dot{C}$ are still given by (5.9) and (5.10) while those of the scalar field are simply $\dot{\phi}=\pi$ and $\dot{\pi}=0$.

## C. Dynamics

The Hamiltonian flow in $\overline{\mathcal{P}}_{\text {red }}$ fully captures the gauge invariant properties of the truncated dynamics of fields at any one fixed spatial point on ${ }^{3} M$. Let us therefore focus on this Hamiltonian system. Although the basic constraint and evolution equations on $\overline{\mathcal{P}}_{\text {red }}$ are

[^5]just ODEs, they have a rich structure; indeed they incorporate the dynamics of all Bianchi Type A models. Since the analysis of Bianchi IX is already quite complicated and required considerable effort [36, 37], we will follow the strategy used in [28] and analyze implications of the reduced equations near fixed points.

There are two sets of fixed points of the dynamics, i.e., points at which $\dot{C}_{I}=\dot{P}_{I}=0$ :

1. $C_{1}=C_{2}, C_{3}=0, P_{1}=P_{2}, P_{3}=0$, and $\pi=0$
2. $C_{I}=0$ and $P_{I} P^{I}-\frac{1}{2} P^{2}+\frac{1}{2} \pi^{2}=0$.

The first set of fixed points corresponds essentially to a dimensional reduction of our theory [38] and is therefore highly unstable. To show that our truncation captures the standard features associated with the BKL behavior near singularities, it will suffice to focus on the second set which, we will now show, in fact corresponds to the Kasner solutions. One can show that the solutions to the scalar constraint $2 P_{I} P^{I}-P^{2}+\pi^{2}=0$ are such that all three $P_{I}$ are positive or all three are negative. Choice of positive signs turns out to be necessary and sufficient for the singularity to appear at $t=+\infty$ as per our previous conventions.

Let us return for a moment to the homogeneous phase space $\mathcal{P}_{\text {hom }}$ and set lapse $N=S_{-1}$, the fiducial scalar density for which $S_{-1} P_{i j}$ is homogeneous, diagonal, with entries $P_{I}$. We can then solve the evolution equation (3.16) for the triad $E_{i}^{a}(t)$ in terms of $P_{I}$. Finally let us set

$$
\begin{equation*}
p_{I}=1-\frac{2 P_{I}}{P} \quad \text { and } \quad \tau=e^{-P t / 2} \tag{5.13}
\end{equation*}
$$

Then the space-time metric computed from $E_{i}^{a}(t)$ is given by

$$
\begin{equation*}
d s^{2}=-d \tau^{2}+\tau^{2 p_{1}} d x_{1}^{2}+\tau^{2 p_{2}} d x_{2}^{2}+\tau^{2 p_{3}} d x_{3}^{2} \tag{5.14}
\end{equation*}
$$

so that the singularity lies at $\tau=0$ (or $t=\infty$ ). By definition, the constants $p_{i}$ satisfy

$$
\begin{equation*}
p_{1}+p_{2}+p_{3}=1 \tag{5.15}
\end{equation*}
$$

and the Hamiltonian constraint

$$
\begin{equation*}
2 P_{I} P^{I}-P^{2}+\pi^{2}=0 \tag{5.16}
\end{equation*}
$$

on $P_{I}$ translates to the familiar quadratic Kasner constraint

$$
\begin{equation*}
p_{1}^{2}+p_{2}^{2}+p_{3}^{2}=1-p_{\phi}^{2} \quad \text { where } \quad p_{\phi}^{2}=\frac{2 \pi^{2}}{P^{2}} \tag{5.17}
\end{equation*}
$$

For each value of $p_{\phi}<1$, these constraints on the $p_{i}$ define a 1-parameter family of solutions, the intersection of a plane with a 2 -sphere. One can check that if $p_{\phi}^{2}>1 / 2$ all the $p_{i}$ are positive while if $p_{\phi}^{2}<1 / 2$ solutions exist only if one of the $p_{i}$ is negative. We will now show that this distinction plays the key role for the stability of the solution.

Let us now move away slightly from a Kasner fixed point $\left(P_{I}, C_{I}\right)$ and consider the Hamiltonian trajectory through the new point $\left(P_{I}^{\prime}, C_{I}^{\prime}\right)$ :

$$
\begin{equation*}
P_{I}^{\prime}=P_{I}+\delta P_{I}, \quad C_{I}^{\prime}=C_{I}+\delta C_{I} \tag{5.18}
\end{equation*}
$$

Then, the evolution equations for the perturbations are of the form

$$
\begin{equation*}
\left(\delta \dot{P}_{I}\right)=\mathcal{O}\left(\delta P^{2}\right) \quad \text { and } \quad\left(\delta \dot{C}_{I}\right)=-N \delta C_{I}\left(P-2 P_{I}\right)+\mathcal{O}(\delta C \delta P) \tag{5.19}
\end{equation*}
$$

For definiteness, let us set $I=1$. Then $P-2 P_{1}=p_{1} P$ and similarly for $I=2,3$. Now $P$ is positive since all three $P_{I}$ are positive. Therefore, if all $p_{i}$ are positive (i.e. if $p_{\phi}^{2}>1 / 2$ ), the evolution equation for $\delta C_{I}$ is of the type $\left(\delta \dot{C}_{I}\right)=$ (negative definite quantity) $\times \delta C_{I}$, whence the perturbation will decay, implying stability. In terms of the canonical variables describing the scalar field, this occurs when the scalar field is large: $4 \pi^{2}>P^{2}$. This stability is in accordance with the Andersson-Rendall results [9] on approach to space-like singularity in presence of a massless scalar field in full general relativity.

Let us now consider the complementary case where $p_{\phi}^{2}<1 / 2$. By the above reasoning, now $\left(P-2 P_{I}\right)$ is negative for some $I$. For definiteness, let us take $P_{1}$ to be the largest of the $P_{I}$ 's initially so that $\left(P-2 P_{1}\right)$ is negative which implies that $C_{1}$ will grow and we have instability. In this case, we cannot use perturbative analysis for the pair $C_{1}, P_{1}$; it is necessary to keep all order terms in $C_{1}$ and $P_{1}$. For simplicity, let us set $C_{2}=C_{3}=0$ initially. Then values of $C_{2}, P_{2}, C_{3}, P_{3}$ will not change during evolution and equations for $C_{1}, P_{1}$ simplify,

$$
\begin{align*}
& \dot{P}_{1}=-N C_{1}^{2}  \tag{5.20}\\
& \dot{C}_{1}=-N C_{1}\left(P_{2}+P_{3}-P_{1}\right)=-N C_{1} P p_{1} \tag{5.21}
\end{align*}
$$

which can be solved exactly to obtain

$$
\begin{align*}
& P_{1}(t)=P_{2}+P_{3}-2 \sqrt{P_{2} P_{3}} \tanh \left(2 \sqrt{P_{2} P_{3}} N\left(t-t_{o}\right)\right) \\
& C_{1}(t)= \pm 2 \sqrt{P_{2} P_{3}} \operatorname{sech}\left(2 \sqrt{P_{2} P_{3}} N\left(t-t_{o}\right)\right) . \tag{5.22}
\end{align*}
$$



FIG. 1: Evolution of each of the three $C_{I}$ in vacuum, starting from a point near the Kasner fixed point surface. Initial data is $C_{1}=1 \times 10^{-7}, C_{2}=2 \times 10^{-7}, C_{3}=2.2 \times 10^{-7}, P_{1}=0.4, P_{2}=0.8$, $P_{3}=0.0686$ ( $C_{1}$ in blue, $C_{2}$ in green, $C_{3}$ in red). Since none of the initial $C_{I}$ vanish, as expected from analytical considerations, there is a series of separate Taub transitions between Kasner states. Time has been rescaled by a power of $1 / 4$ to allow multiple transitions to be shown on a single plot.

These are the Bianchi II solutions written in our variables. Here $C_{1}$, the unstable variable, rapidly increases and then decays to zero. During that time the $P_{1}$ transitions between one Kasner solution to another. In the asymptotic limits we have:

$$
\begin{align*}
& P_{1}(-\infty)=P_{2}+P_{3}+2 \sqrt{P_{2} P_{3}}=\left(\sqrt{P_{2}}+\sqrt{P_{3}}\right)^{2} \\
& P_{1}(+\infty)=P_{2}+P_{3}-2 \sqrt{P_{2} P_{3}}=\left(\sqrt{P_{2}}-\sqrt{P_{3}}\right)^{2} \tag{5.23}
\end{align*}
$$

(In practice the asymptotic limits are achieved quickly, thanks to the hyperbolic functions of time.) The result of the transition is that $P_{1}$, which was originally was the largest of the three $P_{I}$, has transitioned to a lower value. By a change of variables to the $p_{i}$ used in (5.14) it is apparent that the eigenvalue corresponding to the negative exponent $p_{i}$ is the one which has transitioned, and is positive at the end of the transition. Since the singularity lies at $\tau=0$, this means that the initially expanding direction now contracts, and one of the two contracting directions now expands. Indeed, (5.23) is precisely the ' $u$-map' in $p_{i}$ variables.

In this analysis we have made the simplification that initially $C_{2}=C_{3}=0$. If one starts from a generic point in the vicinity of the Kasner fixed point set and still with $P_{1}$ as the largest of the three $P_{I}$ initially, there would again be a transition of the type (5.22). But


FIG. 2: Evolution of each of the three $P_{I}$ in vacuum, starting from a point near the Kasner fixed point surface, with the same initial data as in Fig. $1\left(P_{1}\right.$ in blue, $P_{2}$ in green, $P_{3}$ in red). The largest eigenvalue, $P_{2}$, transits first. After this transition, $P_{1}$ becomes the largest eigenvalue, now making $C_{1}$ unstable. In time all three $P_{I}$ tend to zero. In terms of parameters $p_{i}$ used in the Kasner metric (5.14), the initially expanding direction $p_{2}$ starts contracting at the end of the transition and initially contracting $p_{1}$ starts expanding.
as $P_{1}$ decreases, after a finite time either $P_{2}$ or $P_{3}$ will now be the largest eigenvalue and making the corresponding $C_{I}$ unstable. That pair will then evolve according to (5.22). This general scenario was borne out in a large class of simulations of the reduced equations of motion. Figs 1 and 2 illustrate this dynamical behavior for generic initial data near the Kasner surface. The Taub transitions are easy to see in Fig 2: even though none of the $C_{I}$ are initially zero, the Taub transitions are well described by the analytical expressions (5.22). Fig 3 illustrates the dynamical behavior in cases where the initial data is quite far from the Kasner surface. Note that even in this case, the $C_{I}$ decrease in time so that, although we start far away from the Kasner surface, dynamics drives the state to the Kasner surface.

We can also draw some lessons for the full theory from this behavior of the truncated system. Recall that the dynamical trajectories discussed above can be thought of as representing the evolution of fields at a fixed spatial point. Let us therefore return to ${ }^{3} M$ and consider fields $C_{I}(x), P_{I}(x)$. Now, generically, we will encounter a point $x_{0}$ where the $C^{I}$ all vanish, while being non-zero is the neighborhood of the point. As we noted in section VB , the sign of $C_{I}$ is preserved throughout the evolution. This is in particular true during the Taub transitions where the magnitude of $C_{I}$ grows. Therefore, on 'one side' of $x_{0}$, a


FIG. 3: Evolution of each of the three $C_{I}$ in vacuum, starting from a point away from the Kasner fixed point surface. Initial data are $C_{1}=0.7431, C_{2}=0.3922, C_{3}=0.6555, P_{1}=0.1712$, $P_{2}=0.0 .7060, \quad P_{3}=-0.3140\left(C_{1}\right.$ in blue, $C_{2}$ in green, $C_{3}$ in red). Even though we start out far from the Kasner surface (where all $C_{I}$ vanish), dynamics drives the state to the Kasner surface. Again, time has been rescaled by a power of $1 / 4$ to allow multiple transitions to be shown on a single plot.
$C_{I}$ will positive and increasing in magnitude, while on the 'other side' it will be negative and increasing in magnitude. Therefore its derivative will increase rapidly. Similarly the under Taub transitions the values of $P_{I}(x)$ will change from those of one Kasner solution to another except at the point $x_{0}$. Again, this dynamics will generate a large derivative at $x_{0}$. Thus, analysis of the reduced system suggests that spikes will occur in the full system (3.13) - (3.14). As is well known, these spikes were found in numerical simulations and, more recently, also in analytical treatments [43, 44]. Whenever spikes appear, the key assumption underlying BKL truncation is brought to question because the spatial derivatives are large at the spikes. The key issue for the BKL conjecture - and for the application to quantum gravity we proposed in section I- is whether the time derivatives still dominate generically, as they do in examples.

Let us summarize. Using analytical and numerical methods we showed that there exists a well defined subspace $\mathcal{P}_{\text {hom }}$ of the full phase space $\mathcal{P}$ which exhibits exactly the properties expected in the BKL conjecture. Our procedure to arrive at the reduced system is more direct than those available in the literature. In [28], for example, elimination of the off-
diagonal components and the anti-symmetric parts of $C_{i j}$ involves an additional assumption, beyond ignoring spatial derivatives in favor of time derivatives: these quantities are identified as part of the 'stable subset' (variables that are expected to decay rapidly as the singularity is approached) and then set to zero to obtain the truncated equations. In our treatment, on the other hand, the fact that the antisymmetric part of $C_{i j}$ is negligible is directly implied by the assumption that the $D_{i}$ derivatives are negligible and the constraints imply that the variables $C_{i j}$ and $P_{i j}$ can be simultaneously diagonalized which, furthermore, completely fixes the gauge. Thus, our Hamiltonian framework naturally led to a diagonal gauge, enabling us to quickly zero-in on the essential variables and eliminating the need to keep track of the dynamics of extraneous variables involving frame rotations [28, 29]. Finally, the framework easily led us to the Mixmaster behavior - a series of Bianchi I phases interspersed by Bianchi II transitions. We recovered the 'u-map' for these transitions, and observed the behavior expected from the Andersson and Rendall analysis [9] when a scalar field of large enough magnitude is introduced.

## VI. DISCUSSION

We began with the Hamiltonian formulation of general relativity underlying LQG where the basic fields are spatial triads $E_{i}^{a}$ with density weight 1 , spin connections $\Gamma_{a}^{i}$ they determine, and extrinsic curvatures $K_{a}^{i}$. Based on examples that have been studied analytically and numerically, it seems reasonable to expect that the determinant $q$ of the spatial metric $q_{a b}$ would vanish and the trace $K$ of the extrinsic curvature would diverge at space-like singularities. (This expectation is in particular borne out in the numerical simulations of G2 space-times [33].) One can therefore hope to obtain quantities which remain well-defined at the singularity either by multiplying the natural geometric fields by suitable powers of $q$ or dividing them by suitable powers of $K$. In the commonly used framework due to Uggla et al $[13,28,41]$, one chooses to divide by $K$. One first introduces the so-called Hubble normalized triad $K^{-1} e^{a}{ }_{i}$ by rescaling the orthonormal triad $e_{i}^{a}$ by $K^{-1}$, and then constructs a set of Hubble normalized fields by contracting $\Gamma_{a}{ }^{j}$ and $K_{a}{ }^{j}$ with $K^{-1} e^{a}{ }_{i}$. These fields are expected to have regular limit at the space-like singularity. Einstein's equations expressed in terms of them naturally suggests a truncation and the truncated system successfully describes the expected oscillatory BKL behavior. The resulting form of the BKL conjecture
is supported by numerical evolutions of full general relativity carried out by Garfinkle [39]. However, because there is no underlying Hamiltonian framework, this approach does not easily lend itself to non-perturbative quantization. Even if such a framework were to be constructed, because of the presence of the $K^{-1}$ factor, it would be difficult to introduce quantum operators corresponding to the Hubble rescaled fields.

Motivated by quantum considerations, we adopted the complementary strategy of multiplying geometrical fields by $\sqrt{q}$. The LQG Hamiltonian formulation we began with already features a density weighted triad with exactly the desired property: $E^{a}{ }_{i}=\sqrt{q} e_{i}^{a}$. Since $\sqrt{q}$ is expected to vanish at the singularity, one can hope to use $E_{i}^{a}$ in place of the Hubble normalized $K^{-1} e_{i}^{a}$ to construct a new set of fields to formulate the BKL conjecture. Indeed, (modulo trace terms) our basic variables $C_{i}{ }^{j}$ and $P_{i}{ }^{j}$ were obtained simply by contacting the spatial indices of $\Gamma_{a}{ }^{j}$ and $K_{a}^{j}$ by $E_{i}^{a}$. Furthermore, because $E_{i}^{a}$ vanishes in the limit, the operator $D_{i}:=E_{i}^{a} D_{a}$ provided a key tool in the formulation of the BKL conjecture: asymptotically, $D_{i} C_{j}{ }^{k}$ and $D_{i} P_{j}{ }^{k}$ should become 'negligible' relative to $C_{j}{ }^{k}$ and $P_{j}{ }^{k}$. Now, in exact general relativity, time derivatives of $C_{i}{ }^{j}$ and $P_{i}{ }^{j}$ can be expressed in terms of their $D_{i}$ derivatives, purely algebraic (and at most quadratic) combinations of $C_{i}{ }^{j}$ and $P_{i}{ }^{j}$, the lapse $N$ and its $D_{i}$ derivatives (see (3.6)-(3.15)). Therefore, if in the limit the $D_{i}$ derivatives of the basic fields become negligible compared to the fields themselves, we are naturally led to conclude that time derivatives would dominate the spatial derivatives. This chain of argument led to our formulation of the BKL conjecture.

This rather simple idea depends on the fact that the structure of Einstein's equations has an interesting and unanticipated feature: as we saw in section III, once the triplet $C_{i}{ }^{j}, P_{i}{ }^{j}, D_{i}$ is constructed from the triad $E_{i}^{a}$ and the extrinsic curvature $K_{a}^{i}$ on an initial slice, the constraint and evolution equations can be expressed entirely in terms of the triplet. Given a solution to these equations, the spatial triad $E_{i}^{a}$ (and hence the metric $q_{a b}$ ) can be recovered at the end simply by solving a total differential equation (3.16). This is a surprising and potentially deep property of Einstein's equation. It played essential role in our formulation of the BKL conjecture and could well capture the primary reason behind the BKL behavior observed in examples and numerical simulations.

Since our framework is developed systematically from a Hamiltonian theory, its BKL truncation naturally led to a truncated phase space. The specific truncation used has an important property: The truncated constraint and evolution equations on the truncated
phase space coincide with the truncation of full equations on the full phase space. On the truncated phase space we could solve and gauge-fix the Gauss and vector constraints to obtain a simple Hamiltonian system (which encompasses all Bianchi type A models). Solutions to this system were explored both analytically and numerically. We showed that they exhibit the Bianchi I behavior, the Bianchi II transitions and spikes as in the analysis of symmetry reduced models [45] and numerical investigations of full general relativity [13]. Therefore, as explained in section I, an appropriate quantization of the truncated system, e.g., a la loop quantum cosmology, could go a long way toward understanding the fate of generic space-like singularities in quantum gravity.

In sections III, V A and VB, we restricted ourselves to vacuum equations. The addition of a massless scalar field is straightforward and was carried out in the reduced phase space framework in section VC. If the energy density in the scalar field is small, one again has Bianchi II transitions and spikes. However, once the energy density exceeds a critical value, these disappear and the asymptotic dynamics at any spatial point is described just by the Bianchi I model with a scalar field without transitions. Thus, our truncated system faithfully captures the main features generally expected from the analysis of Andersson and Rendall [9] in full general relativity coupled to a massless scalar field or stiff fluid. Thus, although the initial motivation came from quantum considerations, our formulation of the BKL conjecture, and the form of the field equations both in the full and truncated versions, should be useful also in the analytical and numerical investigations of singularities in classical general relativity.

We will conclude with a discussion comparing our approach with that of Uggla, Ellis, Wainwright and Elst (UEWE) ([28]). The Hubble normalized variable used in their formulation of field equations are give by

$$
\begin{align*}
\Sigma_{i j} & =3 K^{-1} e_{(i}^{a} K_{|a| j)}-K^{-1} e_{k}^{a} K_{a}^{k} \delta_{i j}  \tag{6.1}\\
N_{i j} & =-3 K^{-1} e_{(i}^{a} \Gamma_{|a| j)}+3 K^{-1} e_{k}^{a} \Gamma_{a}^{k} \delta_{i j}  \tag{6.2}\\
A_{i} & =-\epsilon_{i}^{j k} 3 K^{-1} e_{j}^{a} \Gamma_{a}^{k}  \tag{6.3}\\
\partial_{i} & =3 K^{-1} e_{i}^{a} \partial_{a} . \tag{6.4}
\end{align*}
$$

These variables are especially useful because they are scale invariant: they are unchanged under a constant rescaling of the space-time metric. Because of this property and because of the 'regulating' factor $K^{-1}$ in their expressions, it is hoped that in the limit as one approaches
the space-like singularity, these variables will remain finite [41] and their $\partial_{i}$ derivative will become negligible.

We began with quite a different motivation and our focus was on constructing a Hamiltonian framework rather than on differential equations. Since our emphasis was on constructing phase space variables that can be readily promoted to well-defined quantum operators, from the start we avoided the use of factors such as $1 / K$. As a result, our basic variables $C_{i}{ }^{j}$ and $P_{i}{ }^{j}$ are not scale invariant. Could we have made a different choice which is also well suited for quantization and at the same time enjoyed scale invariance? The answer is in the negative for the following reason. Under constant conformal rescalings $g_{a b} \rightarrow \lambda^{2} g_{a b}$ of the space-time metric, we have $E_{i}^{a} \rightarrow \lambda^{2} E_{i}^{a}, \Gamma_{a}^{i} \rightarrow \Gamma_{a}^{i}$, and $K_{a}^{i} \rightarrow K_{a}^{i}$. Now, in the analysis of approach to singularity, scale invariant quantities are directly useful only if they are space scalars and it is not possible to construct scale invariant scalars using just sums of products of these fields, i.e., without introducing fields such as $K^{-1}$ for which it is difficult to construct quantum operators. Even if one introduces additional non-dynamical fields, such as fiducial frames to construct scalars, for natural choices of these frames, scale invariant components of fields such as $K_{a}^{i}, \Gamma_{a}^{i}$ typically diverge at the singularity. Thus, with our motivation, it does not seem possible to demand scale invariance of the basic variables that are to feature in the BKL conjecture.

Our viewpoint is that the most important feature of the Hubble normalized variables is that although the orthonormal triad $e_{i}^{a}$ typically diverges as one approaches a spacelike singularity, $K$ diverges even faster, making the combination $K^{-1} e_{i}^{a}$ go to zero at the singularity. Furthermore, it goes to zero at a sufficient rate for its contraction with $K_{a}^{i}, \Gamma_{a}^{i}$ and $\partial_{a}$ in (6.1) - (6.4) to tame the a priori divergent behavior of these fields. Instead of dividing the orthonormal triad $e_{i}^{a}$ by $K$ which one expects to diverge at the singularity, our strategy was to multiply it by the volume element $\sqrt{q}$ which, in examples, goes to zero at the singularity. This difference persists also in the treatment of the lapse. The UEWE framework assumes that the (scalar) lapse $\bar{N}$ is such that $\bar{N} K$ admits a limit $\underline{\mathrm{N}}$ while we assume that the density weighted lapse $N=(\sqrt{q})^{-1} \bar{N}$ admits a well-defined limit at the singularity. Thus, in both cases, the standard scalar lapse $\bar{N}$ goes to zero so the singularity lies at $t=\infty$.

The key scale invariant UEWE variables $\left(N_{i j}, \Sigma_{i j}\right)$ —which are expected to be well be-
haved at the singularity - are related to our $\left(C_{i j}, K_{i j}\right)$ via

$$
\begin{align*}
N_{i j} & =6 P^{-1} C_{(i j)} & \text { and } & \Sigma_{i j}=-6 P^{-1} P_{(i j)}+2 \delta_{i j}, \quad \text { or, }  \tag{6.5}\\
C_{(i j)} & =-\frac{K \sqrt{q}}{3} N_{i j} & \text { and } & P_{(i j)}=\frac{K \sqrt{q}}{3}\left(\Sigma_{i j}-2 \delta_{i j}\right) \tag{6.6}
\end{align*}
$$

and the two sets of lapse fields are related by:

$$
\begin{equation*}
\underline{\mathrm{N}}=K \sqrt{q} N . \tag{6.7}
\end{equation*}
$$

If one focuses only on the structure of differential equations near space-like singularities, the two reduced systems would in essence be equivalent if $K \sqrt{q}$ admits a finite, nowhere vanishing limit at the singularity. This condition holds for Bianchi I models and also Bianchi II which describe the transitions between Bianchi I epochs. In fact in the Bianchi I model, $\sqrt{q} K=1$ and our density weighted triad has the same dependence on proper time as the Hubble normalized triad. Thus, although the motivations, starting points and procedures used in the two frameworks are quite different, surprisingly, in the end the basic variables and equations are closely related.

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## Appendix A: Densities

Since the basic variables that feature in our formulation of the BKL conjecture are scalars on ${ }^{3} M$ of density weight 1 , in this Appendix we briefly recall a coordinate independent framework for describe densities. The underlying idea is due to Wheeler and the detailed framework was developed by Geroch (see, e.g., [46]). This framework goes hand in had with Penrose's abstract index notation [47, 48]. Because the primary application in this paper is to our fields $C_{i}{ }^{j}, P_{i}{ }^{j}$ on ${ }^{3} M$ we will focus on scalar densities on 3-manifolds. But generalization to tensor densities on n -manifolds is straightforward.

Fix an oriented 3 -manifold ${ }^{3} M$ and fix a orientation thereon. Denote by $\mathcal{E}$ the space of smooth, positively oriented, no-where vanishing, totally skew tensor fields $e^{a b c}$ on ${ }^{3} M$.

Clearly, given any two elements $e^{a b c}$ and $e^{\prime a b c}$ in $\mathcal{E}$, there exists a (strictly) positive function $\alpha$ such that $e^{\prime a b c}=\alpha e^{a b c}$. This fact will be used repeatedly.

In this paper, a scalar density $S_{n}$ of weight $n$ is a map from $\mathcal{E}$ to the space of (real valued) smooth functions on ${ }^{3} M: e \rightarrow S_{n}(e)$, such that:

$$
\begin{equation*}
S_{n}\left(e^{\prime}\right)=\alpha^{n} S_{n}(e) \tag{A1}
\end{equation*}
$$

Here $n$ can be any real number but in most applications in general relativity it is an integer. (In quantum mechanics, on the other hand, states are (complex-valued) densities of weight $1 / 2$ on the configuration space [46].) Since $C_{i}{ }^{j}, P_{i}{ }^{j}$ have density weight 1 , let us make a short detour to discuss the case $n=1$. Fix any 3 -form $s_{a b c}$ on ${ }^{3} M$. It determines a canonical scalar density of weight 1 :

$$
\begin{equation*}
S_{1}(e):=s_{a b c} e^{a b c} \tag{A2}
\end{equation*}
$$

Conversely, since $S_{1}$ is a linear mapping from $\mathcal{E}$ to smooth functions, it determines a canonical 3 -form $s_{a b c}$. Thus, our basic variables could also be taken to be 3 -forms $C^{i j}{ }_{a b c}, P^{i j}{ }_{a b c}$ on ${ }^{3} M$ which take values in second rank tensors in the internal space. The standard ADM phase space of general relativity can be similarly coordinatized by positive definite metrics $q_{a b}$ and tensor fields $P_{c d e}^{a b}$ which are symmetric in $a, b$ and totally skew in $c, d, e[49,50]$. Finally note that every metric $q_{a b}$ determines a canonical volume 3 -form $\epsilon_{a b c}$ which has positive orientation and satisfies $\epsilon_{a b c} \epsilon_{d e f} q^{a d} q^{b e} q^{c f}=\operatorname{sgn}(q)$ 3!. Therefore it also determines a canonical scalar density $\sqrt{q}$ of weight 1 , called the square root of the determinant of $q_{a b}$ : $\sqrt{q}(e):=\epsilon_{a b c} e^{a b c}$ for all $e \in \mathcal{E}$.

This definition can be extended to density weighted tensor fields in an obvious fashion. Note that every ${ }^{3} M$ carries a natural totally skew tensor density $\eta^{a b c}$ of weight 1 , called the Levi-Civita density:

$$
\begin{equation*}
\eta^{a b c}(e)=e^{a b c} \quad \forall e \in \mathcal{E} \tag{A3}
\end{equation*}
$$

Given any metric $q_{a b}$ on ${ }^{3} M$, the square root of its determinant, $\sqrt{q}$, can also be expressed as $\sqrt{q}=\eta^{a b c} \epsilon_{a b c}$.

Finally, given a derivative operator $D_{a}$ on tensor fields on ${ }^{3} M$, we can extend its action on densities $S_{n}$ of weight 1 in a natural manner. $D_{a} S_{n}$ is a 1-form with the same density weight $n$, given by

$$
\begin{equation*}
\left(D_{a} S_{n}\right)(e)=D_{a}\left(S_{n}(e)\right)-n \lambda_{a} S_{n}(e) \quad \forall e \in \mathcal{E} \tag{A4}
\end{equation*}
$$

where the first term on the right hand side is just the gradient of the function $S_{n}(e)$ and the 1-form $\lambda_{a}$ is given by $D_{a} e^{b c d}=\lambda_{a} e^{b c d}$. Therefore the action of the derivative operator $D_{i}$ introduced in the main text is given by:

$$
\begin{equation*}
\left(D_{i} S_{n}\right)(e)=D_{i}\left(S_{n}(e)\right)-n\left(E_{i}^{a} \lambda_{a}\right) S_{n}(e) \quad \forall e \in \mathcal{E} \tag{A5}
\end{equation*}
$$

Since the derivative operator $D_{a}$ we considered ignores internal indices, this equation gives the action of $D_{i}$ on $C_{i}{ }^{j}$ and $P_{i}{ }^{j}$ by regarding these basic fields simply as scalar densities with weight 1 .

## Appendix B: Full Equations of Motion

In the main text we restricted the equations of motion to the case where the shift is zero as is the Lagrange multiplier for the Gauss constraint. In this appendix we give the equations of motion in full generality for both full general relativity and in our reduced system. The full equations of motion for $C$ and $P$ are as follows.

$$
\begin{align*}
& \dot{C}^{i j}=- \epsilon^{j k l} D_{k}\left(N\left(\frac{1}{2} \delta_{l}^{i} P-P_{l}^{i}\right)\right)+N\left[2 C_{k}^{i} P^{|k| j)}+2 C^{[k j]} P_{k}^{i}-P C^{i j}\right]  \tag{B1}\\
&+N^{k} D_{k} C_{i j}+C_{i j} D_{k} N^{k}+C_{i j} \epsilon_{k l m} N^{k} C^{l m} \\
&+\left(C_{i}^{k} \epsilon_{k l j}+C_{j}^{k} \epsilon_{k l i}\right)\left(\Lambda^{l}-N^{m} C_{m l}+\frac{1}{2} C N^{l}\right) \\
&+D_{i}\left(\Lambda_{j}-N^{k} C_{k j}+\frac{1}{2} N_{j} C\right)-D_{k}\left(\Lambda^{k}-N^{l} C_{l}^{k}+\frac{1}{2} C N^{k}\right) \delta_{i j} \\
& \dot{P}^{i j}=\epsilon^{j k l} D_{k}\left(N\left(1 / 2 \delta_{l}^{i} C-C_{l}^{i}\right)\right)-\epsilon^{k l m} D_{m}\left(N C_{k l}\right) \delta^{i j}+2 \epsilon^{j k m} C^{[i k]} D_{m}(N)  \tag{B2}\\
&+\left(D^{i} D^{j}-D^{k} D_{k} \delta^{i j}\right) N+N\left[-2 C^{(i k)} C_{k}^{j}+C C^{i j}-2 C^{[k l]} C_{[k l]} \delta^{i j}\right] \\
&+ N^{k} D_{k} P_{i j}+P_{i j} D_{k} N^{k}+P_{i j} \epsilon_{k l m} N^{k} C^{l m} \\
&+\left(P_{i}^{k} \epsilon_{k l j}+P_{j}^{k} \epsilon_{k l i}\right)\left(\Lambda^{l}-N^{m} C_{m l}+\frac{1}{2} C N^{l}\right)
\end{align*}
$$

In the reduced system the derivative terms are set to zero leading to the following equations of motion for $C$ and $P$.

$$
\begin{align*}
& \dot{C}_{i j}=N\left[2 C_{k(i} P_{j)}^{k}-P C_{i j}\right]+2 \epsilon_{k l(i} C_{j)}^{k}\left(\Lambda^{l}-N^{m} C_{m}^{l}+\frac{1}{2} C N^{l}\right)  \tag{B3}\\
& \dot{P}_{i j}=N\left[-2 C_{i k} C_{j}^{k}+C C_{i j}\right]+2 \epsilon_{k l(i} P_{j)}^{k}\left(\Lambda^{l}-N^{m} C_{m}^{l}+\frac{1}{2} C N^{l}\right) \tag{B4}
\end{align*}
$$

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[^0]:    *Electronic address: ashtekar@gravity.psu.edu
    ${ }^{\dagger}$ Electronic address: adh195@psu.edu
    ${ }^{\ddagger}$ Electronic address: sloan@gravity.psu.edu

[^1]:    ${ }^{1}$ The restriction on topology is made primarily to avoid having to specify boundary conditions and having to keep track of surface terms. There is no conceptual obstruction to removing this restriction (following, for example, the Hamiltonian framework underlying LQC).

[^2]:    ${ }^{2}$ This operator is linear and satisfies the Leibnitz rule. It ignores internal indices (since the action of $D_{a}$ is non-trivial only on tensor indices). However since its action on a function $f$ does not yield the exterior derivative $d f, \tilde{D}_{i}$ is not a connection. If we were to formally treat as a connection, it would have torsion, which is related to $C$ : $\tilde{D}_{[i} \tilde{D}_{j]} f=-\tilde{T}^{k}{ }_{i j} \tilde{D}_{k} f$ where $\tilde{T}^{k}{ }_{i j}=\epsilon_{k l[i} \tilde{C}_{j]}{ }^{l}$. In what follows, $D_{i}$ often acts on scalar densities. This action is given explicitly in Appendix A.

[^3]:    ${ }^{3}$ By their definitions, the internal metric $\stackrel{i}{q}_{i j}$ and the alternating tensor $\epsilon_{i j k}$ are kinematic, fixed once and for all, and are annihilated by all derivative operators $D_{a}$ and $D_{i}$.

[^4]:    ${ }^{4}$ Note that, thanks to the integrals in the definitions of $C_{I}$ and $P^{I}$, the delta-distributions on the right hand side of truncated Poisson brackets (5.1) - (5.2) on $\mathcal{P}$ have now disappeared. To write the truncated constraints (4.3), (4.4) in terms of $C_{I}, P^{I}$, one first fixes a nowhere vanishing scalar density $S_{1}$ of weight 1 (i.e., a 3 -form; see Appendix A). One then multiplies these constraints $\left(S_{1}\right)^{-2}$ to obtain constraints with

[^5]:    density weight zero. Finally, by noting that $C_{1}=\left(C_{1}{ }^{1} S_{-1}\right) V_{o}$, etc, where $V_{o}$ is the volume of ${ }^{3} M$ with respect $\left(S_{1}\right)$, one obtains the equations of motion for $C_{I}, P^{I}$ given below.

