Generating function techniques for loop quantum cosmology

Daniel Cartin[*]

Naval Academy Preparatory School,

197 Elliot Street, Newport, Rhode Island 02841

Gaurav Khanna[†]

Physics Department, University of Massachusetts at Dartmouth,

North Dartmouth, Massachusetts 02747 and

Natural Science Division, Southampton College of

Long Island University, Southampton, New York 11968

Martin Bojowald[‡]

Max-Planck-Institut für Gravitationphysik,

Albert-Einstein-Institut, 14476 Potsdam, Germany

(Dated: July 10, 2004)

Abstract

Loop quantum cosmology leads to a difference equation for the wave function of a universe. In the semiclassical limit, small-scale oscillations must be suppressed by choosing parameters of general solutions appropriately. For anisotropic models this is not possible to do numerically by trial and error; instead, it is shown here for the Bianchi I LRS model how this can be done analytically, using generating function techniques. Those techniques can also be applied to more complicated models, and the results gained allow conclusions about initial value problems and possible large quantum gravity effects.

[*]Electronic address: cartin@naps.edu

[†]Electronic address: gkhanna@umassd.edu

[‡]Electronic address: mabo@aei.mpg.de

arXiv:gr-qc/0405126 v1   26 May 2004

1

I.   INTRODUCTION

One of the two main avenues for current research in quantum gravity is that of quantum geometry (also known as loop quantum gravity). This is a theory that leads to space-time that is discrete at Planck-length scales, giving rise to predictions of quantized areas and volumes (see [1] for reviews). In recent years, these ideas have been applied to the study of cosmology [2]. Just as minisuperspace models reduce the infinitely many degrees of freedom down to a finite, quantum mechanical model, the basic idea of loop quantum cosmology (LQC) is to use symmetry reduction to develop relatively simple models for various space-times. However, many of the features of LQC are similar to those in the full theory; in particular, the Hamiltonian constraint is constructed analogously to the full one [3], and as a consequence takes the form of a discrete recursion relation [4].

Loop quantum cosmological models are free of singularities, irrespective of the type of matter content [5]. This is seen as a general consequence of the quantum evolution equation, which is a difference equation for the wave function and does not break down where the classical singularity would be. At the same time, additional conditions for the wave function can arise which can be interpreted as dynamical initial conditions [6]. For a vacuum isotropic model [7], it turns out that together with the notion of *pre-classicality* [6] a unique LQC solution is picked out. Pre-classicality requires the coefficients of the wave function to lack large variations over Planck-scale lengths, and thus allows the solution to match a semi-classical wave function far away from the singularity. Because one is dealing with discrete recursion relations, this means that as the parameter is increased by one, there should not be a great change in the value of the coefficients. The situation is more complicated in anisotropic models, with several independent directions in minisuperspace along which oscillations need to be suppressed, and therefore the Hamiltonian constraint becomes a partial difference equation. We will look in detail at the Bianchi I LRS model, which has only two independent degrees of freedom and simplifies thanks to its separable evolution equation. As we will see, the generic sequence alternates between positive and negative values, thus exhibiting huge oscillations. However, with the new techniques introduced here to LQC it is possible to select out special boundary values that give pre-classical sequences; from this set of possibilities, pre-classical wave functions can be built up.

To study the relation between the quantum theory and its classical limit, it is of particular

interest to construct solutions which in presumed semiclassical regimes describe wave packets following classical trajectories at least approximately. This requires a sufficiently large set of independent pre-classical solutions such that an initial wave packet can be formed by superposition. That this is realized is not at all obvious. For instance, the continuum limit of the difference equation with the corresponding (DeWitt) initial condition is not well-posed (any solution to the Wheeler–DeWitt equation that is zero at the boundaries of minisuperspace vanishes identically). Even though there are LQC models which are well-posed in contrast to their Wheeler–DeWitt analog [8], it is conceivable that in a model like that studied here the lack of well-posedness in the continuum limit precludes the existence of sufficiently many pre-classical solutions. This indeed turns out to be the case as will be discussed later together with possible consequences and interpretations.

The loop quantized Hamiltonian constraint for the particular case of a Bianchi I LRS space-time used here has already been worked out [9]. Here we present more systematic methods of finding solutions with particular properties, which are useful not only for this space-time, but for any model system to be considered in loop quantum gravity. In Section II, we discuss in detail how to use generating functions to obtain information about a sequence with one parameter. This allows us to tune the magnitude and asymptotic behavior of the sequence by choosing the appropriate initial values. By combining two such one-parameter sequences, we can solve the Bianchi I LRS recursion relation, and pick appropriate combinations to have the desired properties at large values of the evolution parameter n. Section III generalizes the similar method to solve the full two parameter recursion relation. However, because of numerical limitations, the actual sequence is obtained only over a small extent in the parameters m and n, but still its properties can be tuned by appropriate choices of boundary conditions. The general solutions we obtain here are similar in form to those of Section II. As an application of the results we discuss the issue of pre-classical solutions and the semiclassical limit in the Conclusions.

II.   SEPARABLE SOLUTIONS

The Bianchi I LRS (locally rotationally symmetric) model is the simplest anisotropic model, being derived from the Bianchi I model with symmetry group $\mathbb{R}^3$ by imposing the condition of one rotational symmetry. There are thus two degrees of freedom left. In

addition, the classical equations of motion of the model can easily be decoupled, and the quantum Hamiltonian separates. We will first recall the basic equations of this model from the appendix of [9] and then discuss its separated evolution equations.

A. The Bianchi I LRS model

The Bianchi I LRS model has two degrees of freedom which, in real Ashtekar variables, are given by two connection components (A, c) and the conjugate momenta (p_A, p_c) with sympletic structure given by $\{A, p_A\} = \frac{1}{2}\gamma\kappa$ and $\{c, p_c\} = \gamma\kappa$. Here, $\kappa = 8\pi G$ is the gravitational constant and γ the Barbero–Immirzi parameter of loop quantum gravity. The momenta (p_A, p_c) are components of an invariant densitized triad which determine the scale factors a_I of a Bianchi I metric by $a_1 = \sqrt{|p_c|} = a_2$, $a_3 = p_A/\sqrt{|p_c|}$. Thus, the metric is $ds^2 = |p_c|(dx^2 + dy^2) + p_A^2/|p_c|dz^2$ in Cartesian coordinates and is degenerate for $p_A = 0$ or $p_c = 0$.

The behavior of (A, c) and (p_A, p_c) as functions of time is determined by the Hamiltonian constraint

$$H = -\frac{A(2cp_c + Ap_A)}{\sqrt{|p_c|}} \tag{1}$$

which is proportional to $-Ap_A - 2cp_c$, leading to decoupled Hamiltonian equations of motion solved by $p_A \propto \sqrt{\tau}$, $p_c \propto \tau^2$, $A \propto 1/\sqrt{\tau}$, $c \propto 1/\tau^2$. After introducing a new time coordinate $t := \tau^{3/2}$, we obtain $p_A \propto t^{1/3}$ and $p_c \propto t^{4/3}$ and thus scale factors $a_1 = a_2 \propto t^{2/3}$, $a_3 \propto t^{-1/3}$ whose exponents $\alpha_1 = \alpha_2 = 2/3$ and $\alpha_3 = -1/3$ indeed solve the Kasner conditions for Bianchi I solutions, $\sum_I \alpha_I = 1 = \sum_I \alpha_I^2$ in the special LRS case $\alpha_1 = \alpha_2$.

After quantizing the model with loop techniques [9], the triad components p_A and p_c become basic operators with discrete spectra, $\hat{p}_A|m, n\rangle = \frac{1}{4}\gamma\ell_P^2 m|m, n\rangle$ and $\hat{p}_c|m, n\rangle = \frac{1}{2}\gamma\ell_P^2 n|m, n\rangle$. The wave function is thus supported on a discrete minsuperspace, and as a solution to the quantized Hamiltonian constraint subject to a difference equation,

$$d(n)(\tilde{t}_{m-2,n} - 2\tilde{t}_{m,n} + \tilde{t}_{m+2,n}) + 2d_2(m)(\tilde{t}_{m+1,n+1} - \tilde{t}_{m+1,n-1} - \tilde{t}_{m-1,n+1} + \tilde{t}_{m-1,n-1}) = 0, \tag{2}$$

where $\tilde{t}_{m,n}$ are the coefficients of the wave function (rescaled by a factor of the world volume of each basis state). Also we have

$$d(n) = \begin{cases} 0 & n = 0 \\ \sqrt{1 + \frac{1}{2n}} - \sqrt{1 - \frac{1}{2n}} & |n| \geq 1 \end{cases} \tag{3}$$

and

$$d_2(m) = \begin{cases} 0 & m = 0 \\ \frac{1}{m} & m \geq 1 \end{cases} \tag{4}$$

For the remainder of the paper, the parameter n will act as a "time" parameter. Defining $t_{m,n} = \tilde{t}_{m+1,n} - \tilde{t}_{m-1,n}$ ($m \geq 1$), the recursion relation simplifies to

$$d(n)[t_{m+1,n} - t_{m-1,n}] + 2d_2(m)[t_{m,n+1} - t_{m,n-1}] = 0. \tag{5}$$

Note that for typographical simplicity, here and throughout the rest of the paper the notation $t_{m,n}$ and $\tilde{t}_{m,n}$ has been reversed from their use in [9]. Since $\tilde{t}_{m,n}$ includes the volume of each basis state, it follows that $\tilde{t}_{m,n}$ must vanish at the boundaries, $\tilde{t}_{0,n} = 0 = \tilde{t}_{m,0}$. Because of its definition in terms of $\tilde{t}_{m,n}$, the values $t_{0,n}$ are freely specifiable; the boundary condition $\tilde{t}_{0,n} = 0$ is then used in computing $\tilde{t}$ from t via $\tilde{t}_{m+1,n} = t_{m,n} + \tilde{t}_{m-1,n}$. We still must have $t_{m,0} = 0$, which will act as boundary conditions for our sequence.

The continuum limit of the difference equation is obtained at large triad components (or in the $\gamma \to 0$ limit [10]), which implies $m, n \gg 1$ such that the difference operators can be approximated by differentials. One thus arrives at the Wheeler–DeWitt equation

$$\frac{1}{2}p_c^{-1}\frac{\partial^2}{\partial p_A^2}\tilde{\psi}(p_A, p_c) + 2p_A^{-1}\frac{\partial^2}{\partial p_A \partial p_c}\tilde{\psi}(p_A, p_c) = 0. \tag{6}$$

Note that the difference equation (2) for $\tilde{t}_{m,n}$ is of order four, higher than that of the Wheeler–DeWitt equation, which is always second order. This is a consequence of the loop quantization and cannot be avoided. It implies that there are more independent solutions to the discrete equation than the Wheeler–DeWitt equation has; in fact, not all the discrete solutions have a continuum limit. Those which do have such a limit are the pre-classical solutions which do not change rapidly if the discrete labels m and n are increased. It is known that, when boundary conditions are not taken into account, there are always sufficiently many pre-classical solutions for the semiclassical limit to be achieved [11]. In practice, finding those solutions is usually difficult when also boundary conditions have to be taken into account.

Solutions of the Wheeler–DeWitt equation can easily be studied after introducing $\psi(p_A, p_c) := \partial\tilde{\psi}/\partial p_A$ and separating the resulting differential equation $p_A\partial\psi/\partial p_A + 4p_c\partial\psi/\partial p_c = 0$. Writing $\psi(p_A, p_c) = \alpha(p_A)\beta(p_c)$ we obtain the conditions $p_A\alpha' = \lambda\alpha$ and $p_c\beta' = -4\lambda\beta$ solved by $\alpha(p_A) \propto p_A^\lambda$, $\beta(p_c) \propto p_c^{-4\lambda}$. Thus, any non-zero solution ψ diverges

either at the boundary $p_A = 0$ or at the classical singularity $p_c = 0$ unless $\lambda = 0$. For the original wave function $\tilde{\psi} = \int \psi dp_A$ this implies that solutions regular at the boundary are available only for $-1 \leq \lambda \leq 0$. DeWitt's condition $\tilde{\psi}(p_A, 0) = \tilde{\psi}(0, p_c) = 0$ in this model is thus ill-posed since not enough separable solutions for constructing given initial values are available.

The difference equation (5) for $t_{m,n}$ can be solved similarly by assuming that the sequence $t_{m,n}$ is separable into two one-parameter sequences a_m and b_n, i.e. $t_{m,n} = a_m b_n$. This is possible if a_m and b_n satisfy

$$a_{m+1} - a_{m-1} = \frac{2\lambda}{m} a_m, \tag{7a}$$

$$b_{n+1} - b_{n-1} = -\lambda d(n) b_n, \tag{7b}$$

where λ is the separation parameter now for the sequences. Any choice of these two sequences will solve the original recursion relation; because the a_m and b_n relations are second-order, the first two values a_0 and a_1, for example, are enough to describe the rest of the sequence a_m for a particular λ. However, as noted before the order is higher than that of the 1st order separated Wheeler–DeWitt equations and there are additional solutions with large oscillations. For negative λ, for instance, picking any two random values for the boundary data will generically give sequences that alternate between positive and negative values with magnitudes that increase as the parameter (m or n) increases. An example of such a generic choice is shown in Figure 1. Because of this alternation, the wave function will not be smooth at large n and therefore not be pre-classical.

That solutions generically have alternating behavior can be understood as follows: For large m, the right hand side of (7a) is usually small compared to the left hand side such that $a_{m+2} \approx a_m$. The relation between neighboring values, a_{m+1} and a_m, is determined by the initial values a_0 and a_1. Together they determine $a_2 = 2\lambda a_1 + a_0$. For negative λ, and $a_0 = 0$, say, a_2 has the opposite sign from a_1 which translates to a_m having the opposite sign from a_{m+1} for large m and thus alternating behavior. If $a_0 \neq 0$, a_2 may have the same sign as a_1, but still generically oscillations will set in later. Only for positive λ is it easy to suppress the oscillations. However, since λ enters the equation for b_n with the sign reversed, now the b-sequence will develop alternating behavior such that the full solution alternates generically.

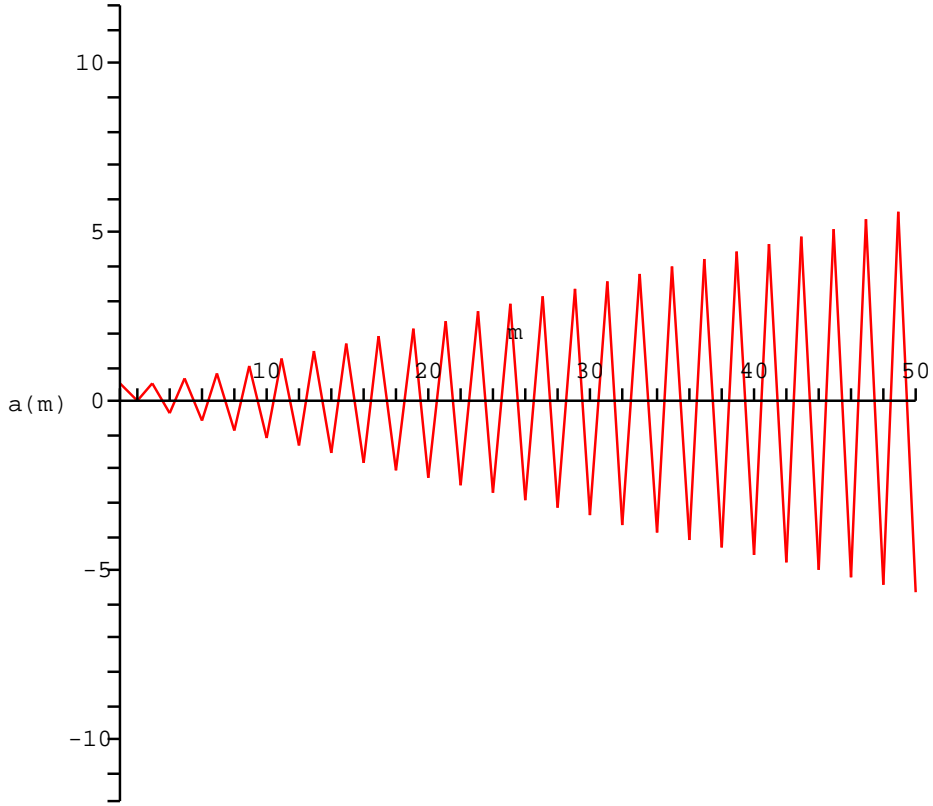We will develop techniques, which can be used analytically or numerically, to check

FIG. 1: Oscillatory behavior of a generic solution to the recursion relation (7a) for the sequence $a_m(\lambda = -1)$. The initial values are $a_0 = a_1 = 1$.

whether it is possible to choose special initial values such that oscillations are suppressed. This will fix the relation between initial values and thus reduce the amount of freedom in pre-classical solutions. In particular, values like a_0 may not be allowed to vanish. While this does not pose a problem for the a-sequence, for the b-sequence we have a different initial value problem, requiring $b_0 = 0$ as a consequence of $t_{m,0} = 0$. Thus, for the b_n the only way to suppress oscillations is by restricting to $\lambda < 0$.

B. Generating functions

Our strategy for choosing the initial values of the sequence a_m will be to work with a generating function[1]. This is a function of one variable x such that the value a_m is the coefficient of x^m in a Taylor expansion, i.e.

$$F(x) = \sum_{m=0}^{\infty} a_m x^m. \tag{8}$$

This will allow us to go from a recursion relation for a_m to a differential equation for $F(x)$. To see how this works, we look at how derivatives act on the function $x^k F(x)$, for a fixed k. We have

$$\frac{\partial}{\partial x}[x^k F(x)] = \sum_{m=0}^{\infty} (m+k) a_m x^{m+k-1}, \tag{9}$$

so we can see that linear functions of m in the recurrence relation become linear derivatives of the generating function. This makes it easier to work with a_m instead of b_n because $d_2(m)$, unlike $d(n)$, is polynomial and the map between recursion relation and differential equation is more obvious. Techniques for studying the values of the b_n sequence will be discussed later.

We start with the recursion relation (7a) for a_m, multiply it by mx^{m-1} and sum over all values of m for which the relation is valid (i.e. $m \geq 0$); then the sum is written as[2]

$$\sum_{m=0}^{\infty} [(m+1)a_{m+2} - 2\lambda a_{m+1} - (m+1)a_m]x^m = 0. \tag{10}$$

By mapping instances of m into derivatives, we arrive at the differential equation for $F(x)$ given by

$$\frac{d}{dx}\left[\frac{F(x) - a_0}{x} - xF(x)\right] - 2\lambda \frac{F(x) - a_0}{x} = 0 \tag{11}$$

or

$$\frac{d}{dx}\left[\frac{1 - x^2}{x}F(x)\right] - 2\lambda \frac{F(x)}{x} + a_0 \frac{1 + 2\lambda x}{x^2} = 0. \tag{12}$$

As written, this equation has singularities at $x = -1, 0$ and 1, which makes it problematic to expand around $x = 0$ in the Taylor series expansion (8) of the generating function; however,

---

[1] For a good reference on generating functions, see Wilf [12]; the related notion of Z-transforms is covered in, e.g., Oppenheim and Schafer [13].

[2] We start the sum at $m = 0$, so that all coefficients are of the form a_{m+k}, instead of beginning at $m = 1$ (with a a_{m-1} term) to avoid placing extra relations on the coefficients a_m. This has the effect of shifting $m \to m+1$.

we are interested not in the solution itself, but in the relation between the coefficients in its series expansion. Because of this, there is some freedom to find an equation more tractable to analysis, so it is natural to define a new function

$$G(x) = \frac{F(x) - a_0}{x}. \tag{13}$$

Substituting this in to the relation for $F(x)$ gives a simpler differential equation for $G(x)$,

$$\frac{d}{dx}\left[(1 - x^2)G(x)\right] - 2\lambda G(x) = a_0. \tag{14}$$

By going from $F(x)$ to $G(x)$, we have reduced the number of singularities by one, but the question now is to relate this new generating function to the sequence a_m. If we take

$$G(x) = \sum_{m=0}^{\infty} \alpha_m x^m, \tag{15}$$

then the mapping (13) between the generating functions $F(x)$ and $G(x)$ implies that the two sequences a_m and α_m are related by

$$a_m = \alpha_{m-1}, \qquad \text{for } m \geq 1. \tag{16}$$

Thus, simplifying the differential equation has resulted in a "shift" upward in the sequences. Once we know the two initial values of the α_m sequence, $\alpha_0(= a_1)$ and $\alpha_1(= a_2)$, then we can find those of the a_m sequence by using

$$\alpha_1 - a_0 = 2\lambda\alpha_0. \tag{17}$$

which comes from the recursion relation (7a) for a_m in the particular case $m = 1$. Thus, the relation between α_0 and α_1 implies one between a_0 and a_1. The information in this differential equation is equivalent to that in the recurrence relation; any series solution of the differential equation (14) will solve the relation (7a) for a_m, after shifting α_m back to a_m via (16).

C. Asymptotic behavior

The question now is how to avoid alternating oscillatory behavior in the sequence. We look at the function $(1 - x)G(x)$, which is a function that generates the *differences* between adjacent values of α_m, that is,

$$(1 - x)G(x) = \alpha_0 + \sum_{m=0}^{\infty}(\alpha_{m+1} - \alpha_m)x^{m+1}.$$

If this function has no singularities, then the sequence α_m will converge to a finite value without oscillation. Because of the $(1 - x^2)$ factor appearing in the differential equation (14) for $G(x)$, the function will in general have poles at $x = \pm 1$. Thus the function is regular for $|x| < 1$, and if there is no singularity at $x = 1$, we have $(1 - x)G(x)|_{x=1} = \alpha_0 + \sum_{m=0}^{\infty}(\alpha_{m+1} - \alpha_m) = \lim_{m \to \infty} \alpha_m$ such that the sequence α_m has a finite limit. Moreover, if there is not a pole at $x = -1$, $\lim_{m \to \infty}(\alpha_{m+1} - \alpha_m) = 0$, so alternating oscillations are suppressed. This avoids situations such as that seen, for example, in the Taylor expansion of $(1 + x)^{-1}$, where the coefficients of x^m alternate sign:

$$\frac{1}{1 + x} = 1 - x + x^2 - x^3 + \cdots . \tag{18}$$

Obviously, $(1 - x)G(x)$ will have the same behavior at $x = -1$ that $G(x)$ does; we avoid oscillations by requiring no singularity in the function $G(x)$ at $x = -1$. From this, we get a relation between the two initial values α_0 and α_1. The story is slightly different at $x = 1$; $G(x)$ may blow up there, but $(1 - x)G(x)$ can be finite if, e.g., $G(x)$ has a simple pole at $x = 1$. Two examples of this are seen in the expansions for $(1 - x)^{-1}$,

$$\frac{1}{1 - x} = 1 + x + x^2 + x^3 + \cdots ,$$

and $\ln(1 - x)$,

$$-\ln(1 - x) = x + \frac{1}{2}x^2 + \frac{1}{3}x^3 + \cdots .$$

In the first, the coefficients of the sequence maintain a constant value; in the second, they converge to zero. We will see that the latter is exactly the behavior found generically in the solutions $G(x)$ for negative λ.

With this in mind, we take as a particular example the choice $\lambda = -1$; solving our differential equation for the generating function $G(x)$ given in (14) with the condition $G(0) = \alpha_0$, we obtain the solution

$$G(x) = \frac{\alpha_0 - (2\alpha_0 + \alpha_1)x - (4\alpha_0 + 2\alpha_1)\ln(1 - x)}{(1 + x)^2}. \tag{19}$$

In obtaining this solution from the differential equation (14) for $G(x)$, we have used the relation (17) between a_0 and the initial values α_0 and α_1. For generic values α_0 and α_1, this function will have singularities at $x = \pm 1$; to ensure that the singularity at $x = -1$ does not give rise to oscillatory behavior at large m, we require that

$$\lim_{x \to -1}[(1 - x)(1 + x)^2 G(x)] = 0. \tag{20}$$

When we solve this relation, we find that

$$\alpha_1 = \left(\frac{4\ln 2 - 3}{2\ln 2 - 1}\right)\alpha_0$$

which already implies that $(1 - x)G(x)$ is regular at $x = -1$. Notice that the $x = 1$ singularity remains because of the $\ln(1 - x)$ term; however, $(1 - x)\ln(1 - x)$ is zero at $x = 1$, so $(1 - x)G(x)$ is regular. As discussed above, this is a "good" singularity where the coefficients of the Taylor series go as $1/m$; this behavior in a_m is seen in Figure 2. We remark here, however, that only for negative λ do we get the type of behavior seen above; when $\lambda > 0$, the pole at $x = 1$ is of higher order.
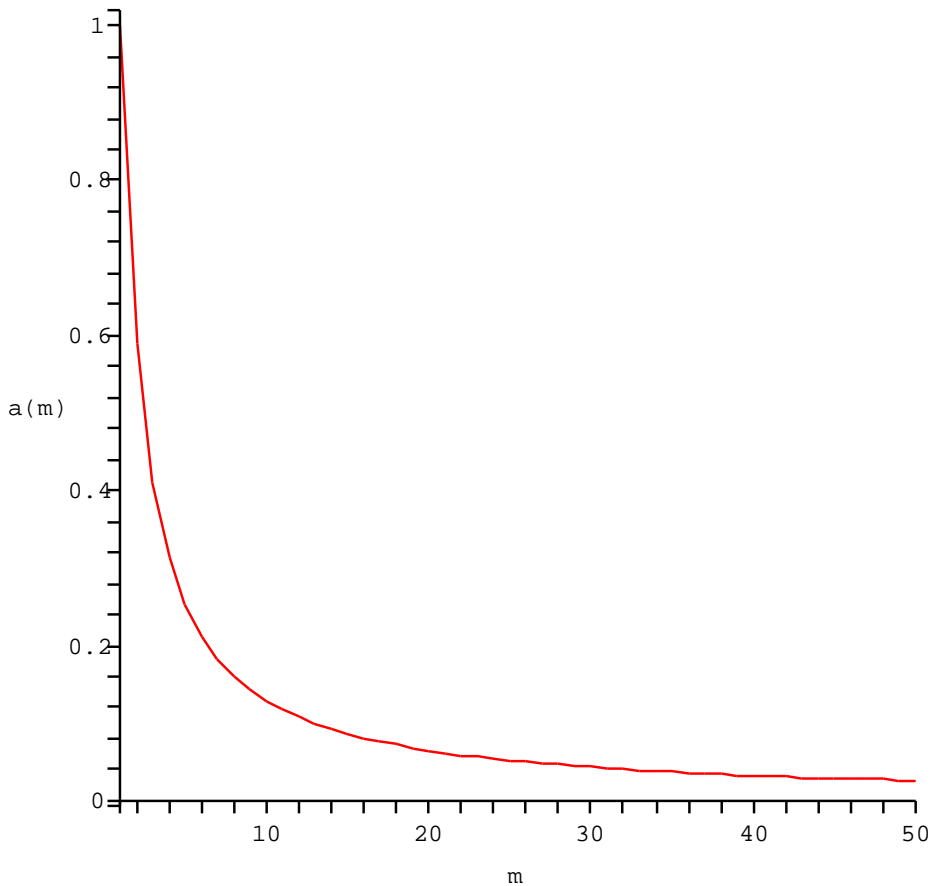

FIG. 2: Values of the sequence $a_m(\lambda = -1)$ where the initial values are chosen to satisfy $(4\ln 2 - 3)\alpha_0 = (2\ln 2 - 1)\alpha_1$. This ensures the sequence converges to a constant value at large m.

For arbitrary λ we first solve the homogeneous equation (14) for $a_0 = 0$ by $G(x) = c(1 + x)^{\lambda-1}(1 - x)^{-\lambda-1}$. By varying the constant c we obtain the general solution to the

11

inhomogeneous equation as

$$G(x) = c(x)(1+x)^{\lambda-1}(1-x)^{-\lambda-1} \tag{21}$$

with

$$c(x) = a_0 \int^x \left(\frac{1-t}{1+t}\right)^\lambda dt = c_0 - \frac{2^\lambda a_0}{\lambda-1}(1+x)^{1-\lambda}{}_2F_1(1-\lambda,-\lambda;2-\lambda;(1+x)/2) \tag{22}$$

for $\lambda \neq 1$ in terms of the hypergeometric function ${}_2F_1$. (If $\lambda = 1$, the equation can be integrated in a manner similar to the $\lambda = -1$ case.) This gives

$$G(x) = c_0(1+x)^{\lambda-1}(1-x)^{-\lambda-1} - \frac{2^\lambda a_0}{\lambda-1}(1-x)^{-\lambda-1}{}_2F_1(1-\lambda,-\lambda;2-\lambda;(1+x)/2) \tag{23}$$

where only the first term determines the singularity structure at $x = -1$ since the hypergeometric function ${}_2F_1(a,b;c;z)$ is regular at $z = 0$ taking the value ${}_2F_1(a,b;c;0) = 1$ for all a,b,c. Thus, the singularity at $x = -1$ can always be removed by choosing $c_0 = 0$. Since

$$a_1 = \alpha_0 = G(0) = c_0 - 2^\lambda a_0/(\lambda-1){}_2F_1(1-\lambda,-\lambda;2-\lambda;1/2)$$
$$= c_0 + a_0 - \lambda a_0(\psi(1/2-\lambda/2) - \psi(1-\lambda/2))$$

with the digamma function $\psi(z) = d\Gamma(z)/dz$, this translates to the condition

$$a_1 = a_0(1 - \lambda(\psi(1/2-\lambda/2) - \psi(1-\lambda/2))). \tag{24}$$

This expression is finite for all λ which are not positive integers since the digamma function is analytic except for simple poles at $-z \in \mathbb{N}$. For $\lambda = -1$, for instance, we can use $\psi(1) - \psi(3/2) = 2\ln 2 - 2$ and re-obtain the special case studied before.

At $x = 1$, ${}_2F_1(a,b;c;(1+x)/2)$ has a branch point which is logarithmic for $c - a - b \in \mathbb{Z}$ or $c - a - b \notin \mathbb{Q}$. Thus, $(1-x)G(x)$ always has a singularity at $x = 1$, which for positive λ is enhanced by the factor $(1-x)^{-\lambda-1}$. Thus, for $\lambda > 0$ the sequence α_m is unbounded.

Now we turn to putting the a_m and b_n sequences back together. For each λ, a pre-classical sequence $t_{m,n}$ – when the boundary values have been appropriately tuned – is completely characterized by the choice of λ, with an additional scaling factor. Because $b_0 = 0$ by the boundary conditions on the sequence, changing b_1 will simply scale the magnitude of the b_n values. Similarly, pre-classicality requires a relation between a_0 and a_1, so one is fixed by the choice of the other, while varying this choice will again only scale the a_m sequence. Since increasing b_1 by a constant factor and decreasing both a_0 and a_1 by the
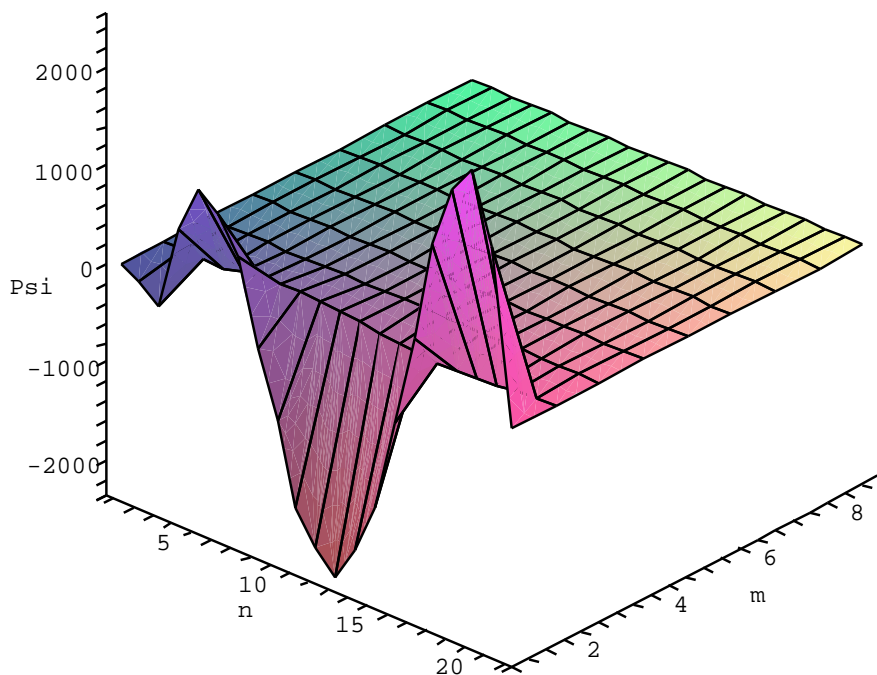
FIG. 3: Values of the sequence $t_{m,n}$ where a linear combination of solutions $a_m b_n$ were chosen such that the wave function evolves into a Gaussian wave packet at large n.

same factor (to preserve their relationship) leaves the $t_{m,n}$ sequence constant, only one of these is independent. Thus, a general pre-classical solution $t_{m,n}$ can be written as a sum $\sum_{\lambda \leq 0} c(\lambda) t_{m,n}(\lambda)$, with the coefficient $c(\lambda)$ used to scale the individual terms of the sum. We can use linear combinations of these to get a generic solution. As an example of this, we require that the sequence $t_{m,n}$ match a Gaussian wave packet in the parameter m, at large values of n (see Figures 3 and 4). One difficulty in doing this, however, is apparent when looking at the a_m graph, Figure 2; because the sequence becomes essentially constant for large m, it is difficult to get the necessary discrimination in m for the wave packet[3].

---

[3] Recall that the sequence $t_{m,n}$ was the "m derivative" of the original sequence $\tilde{t}_{m,n}$, so one might wonder if these conclusions change when $\tilde{t}_{m,n}$ is used. In fact, they remain much the same – since a_m gives the
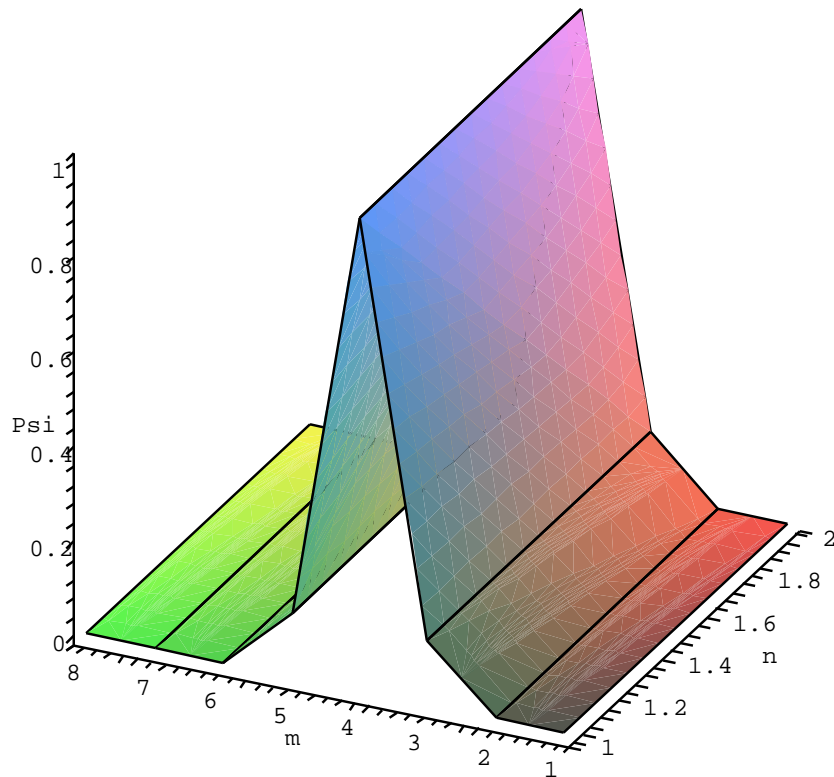
FIG. 4: Close-up of the sequence given in Figure 3, showing the Gaussian wave packet at large values of n.

III.   GENERAL SOLUTIONS

In the previous section, we looked at separating out the m and n dependence into two distinct sequences, then using generating function methods to analyze the a_m sequence. Because this has reduced the problem to finding the right initial values a_0 and a_1, there is much to be said for the simplicity of this method. However, we can ask whether the full recursion relation (5) is amenable to study by generating functions. We shall see that this is feasible, and provides a method to study other spacetimes where the recursion relation

change in $\tilde{t}_{m,n}$ with m, its decline to zero means that $\tilde{t}_{m,n}$ is basically constant for large m. Thus, again only at small m is the spatial discrimination possible to build a wave function with desired properties at large n.

may not be separable (which includes the Schwarzschild black hole interior [14]).

Starting again with the general difference equation (5), we can work with a generating function $F(x, y)$, which describes the sequence. Because occurrences of n translate to derivatives $\partial/\partial y$ of the generating function, the function $d(n)$ on the surface presents a problem – there would be a non-polynomial function of derivatives acting on the generating function. To deal with this, we write the sequence $t_{m,n}$ as

$$t_{m,n} = \sum_{k=0}^{\infty} t_{m,n}^{(k)}, \tag{25}$$

where the $t_{m,n}^{(k)}$ satisfy

$$\frac{1}{2n}[t_{m+1,n}^{(0)} - t_{m-1,n}^{(0)}] + \frac{2}{m}[t_{m,n+1}^{(0)} - t_{m,n-1}^{(0)}] = 0 \tag{26a}$$

$$\frac{1}{2n}[t_{m+1,n}^{(k)} - t_{m-1,n}^{(k)}] + \frac{2}{m}[t_{m,n+1}^{(k)} - t_{m,n-1}^{(k)}] = \left(\frac{1}{2n} - d(n)\right)(t_{m+1,n}^{(k-1)} - t_{m-1,n}^{(k-1)}). \tag{26b}$$

Here, we are using the fact that $d(n) \simeq 1/2n$ to write the sequence $t_{m,n}$ as a perturbation series. In other words, we choose the leading order sequence $t_{m,n}^{(0)}$ to satisfy a recursion relation with coefficients polynomial in the parameters m and n, such that a partial differential equation can be found that is equivalent to the $t_{m,n}^{(0)}$ relation (26a). Boundary or initial values would then be set such that $t^{(0)}$ is pre-classical, i.e. by removing singularities of the generating function. For higher terms $t^{(k)}$, $k \geq 1$, we can choose vanishing boundary and initial values. Each such contribution by itself would not be pre-classical, but its oscillations would contribute only small perturbations to $t^{(0)}$. Indeed, because of the small difference between $1/2n$ and $d(n)$, the right hand side of the equations for $t_{m,n}^{(k)}$, $k > 0$ is suppressed by a factor of n^{-3} compared to the left hand side. It is thus consistent with pre-classicality to use the relation for $t^{(0)}$ in order to fix boundary values as before, and then solve the relations for higher $t^{(k)}$ with boundary and initial values zero. With a vanishing right hand side the solution would be $t_{m,n}^{(k)} = 0$ for $k \geq 1$, and the small right hand side will lead to small values for the higher terms which become negligible compared to the $t_{m,n}^{(0)}$ values. Because of this, for the rest of the paper we focus on solving for the sequence $t_{m,n}^{(0)}$; obtaining finer accuracy for small m, n would be possible using higher $t_{m,n}^{(k)}$

Working with the $t_{m,n}^{(0)}$ sequence, we look for a partial differential equation for the generating function

$$F(x, y) = \sum_{m=0}^{\infty}\sum_{n=0}^{\infty} t_{m,n}^{(0)} x^m y^n. \tag{27}$$

15

Multiplying the recursion relation (26a) for $t_{m,n}^{(0)}$ by $(1/2)mnx^{m-1}y^{n-1}$ and summing over all values it is valid gives

$$\sum_{m=0}^{\infty}\sum_{n=0}^{\infty}\left[\frac{1}{4}(m+1)(t_{m+2,n+1}^{(0)} - t_{m,n+1}^{(0)}) + (n+1)(t_{m+1,n+2}^{(0)} - t_{m+1,n}^{(0)})\right]x^m y^n = 0, \tag{28}$$

and we arrive at an equation for $F(x,y)$ which is similar in form to the separable case, i.e. there are singularities at $x, y = 0$. To avoid this, we define a new function $G(x,y)$ as

$$G(x,y) = \frac{1}{xy}\left[F(x,y) - \sum_{n=1}^{\infty}t_{0,n}^{(0)}y^n\right] = \frac{[F(x,y) - yA(y)]}{xy}, \tag{29}$$

where

$$A(y) = \sum_{n=1}^{\infty}t_{0,n}^{(0)}y^{n-1} \tag{30}$$

is related to the generating function of the $m = 0$ boundary for the original $t_{m,n}^{(0)}$ sequence (the definition of $A(y)$ chosen here is to simplify the form of our eventual differential equation for $G(x,y)$). This sum begins at $n = 1$, since the boundary conditions imply $t_{0,0}^{(0)} = 0$. This gives a "shifted" sequence, since

$$F(x,y) = xyG(x,y) + yA(y). \tag{31}$$

Note the similarity between this relation between $F(x,y)$ and $G(x,y)$, and the analogous one between $F(x)$ and $G(x)$ in the separable case. Again, the coefficients are shifted by one, now in each of the parameters; if

$$G(x,y) = \sum_{m=0}^{\infty}\sum_{n=0}^{\infty}\rho_{m,n}x^m y^n \tag{32}$$

then

$$t_{m,n}^{(0)} = \rho_{m-1,n-1}. \tag{33}$$

This gives us the PDE

$$\frac{1}{4}\frac{\partial}{\partial x}[(1-x^2)G(x,y)] + \frac{\partial}{\partial y}[(1-y^2)G(x,y)] = A(y). \tag{34}$$

Again, we will have singularities at both $x = \pm 1$ and $y = \pm 1$.

Our discussion of the singularities in Section II for separable solutions carries over here similarly for functions of two variables. First, we want the functions $(1 - x)G(x,y)$ and $(1-y)G(x,y)$ both to be finite for all values of x and y, respectively, to ensure that at large

16

m or n, the sequence is either constant or smoothly changing. Putting these together means that $(1-x)(1-y)G(x, y)$ has to be finite for all x, y. As with the separable solutions, the only problem with this might be at $x = -1$ and $y = -1$. One condition for $(1 - x)(1 - y)G(x, y)$ to be finite along these two lines in the $x - y$ plane is that the function

$$H(x, y) = (1 - x^2)(1 - y^2)G(x, y) \tag{35}$$

satisfies $H(-1, y) = H(x, -1) = 0$. When we solve for $G(x, y)$ in terms of $H(x, y)$ in the above relation (35), we find the new equation

$$\frac{1}{4}(1 - x^2)\frac{\partial H(x, y)}{\partial x} + (1 - y^2)\frac{\partial H(x, y)}{\partial y} = (1 - x^2)(1 - y^2)A(y). \tag{36}$$

So, given our boundary conditions on $H(x, y)$ mentioned above, and any choice for $A(y)$, we can solve this equation numerically.

This is exactly how we would go about finding the sequence if there was a desired sequence of values $t_{0,n}$, which is what $A(y)$ specifies. However, more likely one wants a particular limiting case for the sequence $t_{m,n}$ for large n, for example. Here, the properties of the functions $G(x, y)$ and $H(x, y)$ come into play. Because it is assumed that $(1-x)(1-y)G(x, y)$ is finite, then $G(x, y)$ itself can have simple poles at $x = 1$ and $y = 1$. For the cases mentioned in Section II – the functions $(1 - x)^{-1}$ and $\ln(x - 1)$ – the coefficients in the Taylor series converge to constant values (unity in the first sequence, zero in the second). So, if one looks at the expansion in y, the coefficients of $G(x, y)$ will assume some constant profile in x for large powers y^n; this profile will be determined by, e.g., the residue of the function $G(x, y)$ at a simple pole $y = 1$. Up to a constant factor, this is simply the function $H(x, 1)$; along the lines $x = 1$ and $y = 1$, the function $H(x, y)$ gives us information about the asymptotic behavior of the sequence $t_{m,n}$. In fact, $H(x, 1)$ is simply the generating function reflecting how $t_{m,n}$ behaves at large n, and similarly for $H(1, y)$. Thus, to assemble the desired profile at, say, large n, one requires that $H(x, 1)$ be a certain function, treating the y^n coefficients of the source term $A(y)$ as unknowns to be solved for. This can be done either numerically or by using pseudo-spectral methods; the form of the partial differential equation makes it particularly amenable to the use of Chebyshev polynomials. An example of this is shown in Figure 5; notice that this has the same basic shape as the sequence assembled out of the separable solutions in Section II.
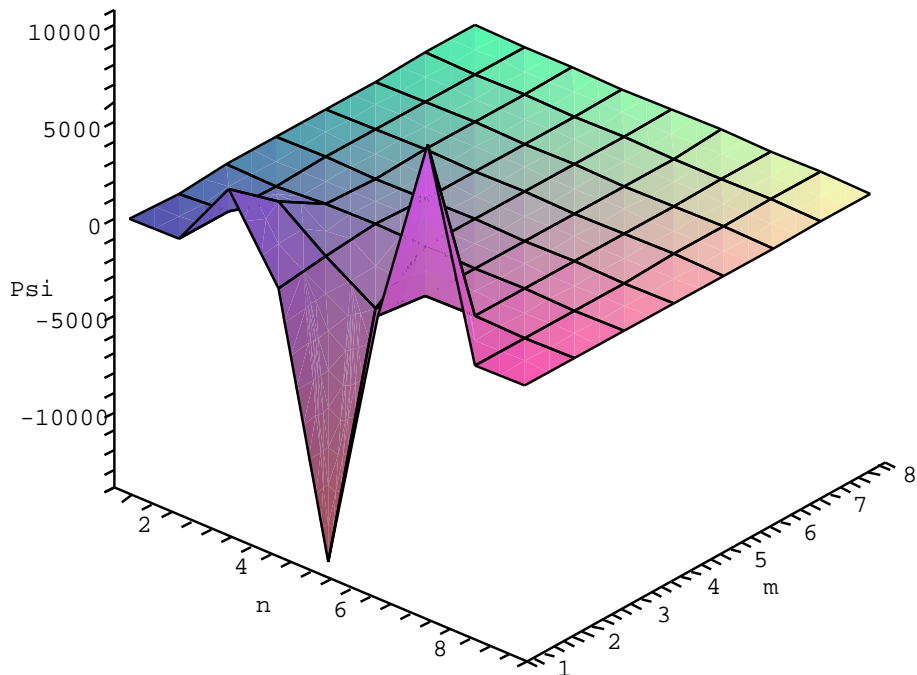
FIG. 5: Values of the sequence $r_{m,n}$ obtained from the Taylor expansion of the generating function $G(x,y)$. Notice the similarity in shape with Figure 3 obtained by combining the one-parameter sequences a_m and b_n.

IV. CONCLUSIONS

Loop quantum cosmology has discrete evolution equations of higher order than the Wheeler–DeWitt differential equation which is obtained in a continuum limit. There are thus additional independent solutions which display an alternating behavior. For studying the semiclassical limit of those models it is important to have control on those solutions for which the small-scale oscillations are suppressed. As demonstrated here for the Bianchi I LRS model, acceptable solutions can be extracted analytically by employing generating function techniques.

For this particular model we can apply the results to discuss the initial value problem. In general, one would need separated solutions for all values of the separation parameter in order to construct a given initial wave packet at large n, far away from the classical singularity at $n = 0$. The Wheeler–DeWitt equation with DeWitt's initial conditions does not allow sufficiently many solutions and thus presents an ill-posed initial value problem. For the difference equation of loop quantum cosmology, the initial value problem is well-posed in the sense that there are always non-trivial solutions. However, in the semiclassical limit one also has to find enough solutions which do not oscillate strongly at small scales. One may then speculate that analogously to the ill-posed Wheeler–DeWitt problem there are not sufficiently many pre-classical solutions. Another system which is ill-posed from the Wheeler–DeWitt point of view, an isotropic model with a free, massless scalar has been studied in [8]. There it turned out that the loop problem is well-posed and still allows enough pre-classical solutions. However, the situation there was different in that the matter term was responsible for the ill-posedness of the continuum formulation. The Bianchi I LRS model thus presents a qualitatively different system to study well-posedness, which can be done in detail with the methods developed in this paper.

What we have seen is that for negative separation parameter λ we can find pre-classical solutions. The problems of the Wheeler–DeWitt quantization at the boundary $p_A = 0$ do not occur in the discrete formulation and pre-classicality puts strong restrictions on the sequence a_m fixing its boundary values. The sequence b_n has only small oscillations for $\lambda < 0$ such that one can choose a pre-classical solution.

For positive λ, on the other hand, the situation is different. Now, the a_m sequence is not problematic, and for b_n one would have to choose special initial values in order to guarantee pre-classicality. However, since $b_0 = 0$ is required by the difference equation, this option is not available and b_n will always be alternating for positive λ. Thus, b_n does not have a continuum limit but $(-1)^n b_n$ does. However, the corresponding continuum limit of the difference equation acting on $(-1)^n a_m b_n$ has an additional relative minus sign from the $(-1)^n$ such that one obtains a different Wheeler–DeWitt equation: Introducing $T_{m,n} := (-1)^n t_{m,n}$ into the difference equation (5) for $t_{m,n}$, we obtain

$$(-1)^n d(n)(T_{m+1,n} - T_{m-1,n}) + 2d_2(m)((-1)^{n+1} T_{m,n+1} - (-1)^{n-1} T_{m,n-1})$$

$$= (-1)^n [d(n)(T_{m+1,n} - T_{m-1,n}) - 2d_2(m)(T_{m,n+1} - T_{m,n-1})] = 0$$

19

where the sign of the second term is switched. This is an example of different continuum limits obtained from one and the same difference equation, which, from the point of view of the discrete formulation, can be interpreted as a duality between different continuum formulations [4].

In order to construct semiclassical wave packets at large n, one can try to use only negative λ in order to avoid oscillations. However, the resulting solutions are mostly concentrated at small values of m since the pre-classical separable solutions a_m decrease with m. One can also see that using only negative λ is not enough by observing that the Wheeler–DeWitt solutions p_A^λ for positive integer λ are just what one needs for a Taylor expansion from which one could construct any analytical initial wave packet. Using these λ in the discrete case requires to have alternating b_n, which implies that such wave packets do not follow the classical trajectory since they are solutions to the Wheeler-DeWitt equation with a sign flip.

Thus, in this model the discrete analog of DeWitt's initial condition may be problematic. It is possible to avoid DeWitt's initial condition by using a symmetric version of the constraint (which is non-singular if the constraint is symmetrized after multiplying with $\text{sgn}(n)$ [7]). In this way detailed studies of models can teach lessons for the full theory since the same ordering should be used in all cases. With this symmetric ordering, b_0 would be free such that it can be fixed as done for the a_m sequence if one requires a pre-classical solution. However, due to the symmetrization of the constraint operator the difference equation will change and be more complicated; moreover, one loses conditions on the wave function. Even with the non-symmetric constraint used here, it follows from the results of this paper that, with the condition of pre-classicality in addition to dynamical initial conditions, the wave function will not be unique.

Alternatively, one can take the lack of pre-classical solutions seriously for this model. If we only look at large values of m and n, i.e. only at the semiclassical regime, there is no problem at all and we can construct any initial state we like. Most of those states would not solve the initial conditions imposed by the quantum constraint at the classical singularity and thus have to be discarded. At this point, however, we already use information from the quantum theory: the behavior of the wave function at the classical singularity is invoked. Thus, the properties of wave functions discussed here can be interpreted as a quantum effect. The fact that this effect can have implications for the propagation of wave packets even far away from the quantum regime suggests possible large quantum gravity effects that should

be studied further. In particular, one has to see what the behavior is in other models, for which the methods described here may prove helpful.

Acknowledgments

[1] C. Rovelli, *Quantum Gravity* (Cambridge University Press, Cambridge, in press);
T. Thiemann, *Introduction to Modern Canonical Quantum General Relativity*, pre-print `gr-qc/0110034`;
A. Ashtekar and J. Lewandowski, Background independent quantum gravity: A status report, pre-print `gr-qc/0404018`

[2] M. Bojowald and H. Morales-Técotl, Lect. Notes Phys. (to appear); pre-print `arXiv:gr-qc/0306008`;
M. Bojowald, Pramana (to appear); pre-print `arXiv:gr-qc/0402053`

[3] T. Thiemann, Class. Quantum Grav. **15**, 839 (1998); pre-print `arXiv:gr-qc/9606089`

[4] M. Bojowald, Class. Quantum Grav. **18**, 1071 (2001); pre-print `arXiv:gr-qc/0008053`

[5] M. Bojowald, Phys. Rev. Lett. **86**, 5227 (2001); pre-print `arXiv:gr-qc/0102069`

[6] M. Bojowald, Phys. Rev. Lett. **87**, 121301 (2001); pre-print `arXiv:gr-qc/0104072`;
M. Bojowald, Gen. Rel. Grav. **35**, 1877 (2003); pre-print `arXiv:gr-qc/0305069`

[7] M. Bojowald, Class. Quantum Grav. **19**, 2717 (2002); pre-print `arXiv:gr-qc/0202077`

[8] M. Bojowald and F. Hinterleitner, Phys. Rev. D **66**, 104003 (2002); pre-print `arXiv:gr-qc/0207038`

[9] M. Bojowald, Class. Quantum Grav. **20**, 2595 (2003); pre-print `arXiv:gr-qc/0303073`

[10] M. Bojowald, Class. Quantum Grav. **18**, L109 (2001); pre-print `arXiv:gr-qc/0105113`

[11] M. Bojowald and G. Date, Class. Quantum Grav. **21**, 121 (2004); pre-print `arXiv:gr-qc/0307083`

[12] H. Wilf, *Generatingfunctionology* (Academic, New York, 1993); available online at the author's website `http://www.cis.upenn.edu/~wilf/`

[13] A. V. Oppenheim and R. W. Schafer, *Digital Signal Processing* (Prentice-Hall, Englewood Cliffs, 1975), Chap. 2

[14] A. Ashtekar and M. Bojowald, in preparation