Interpretation of the triad orientations in loop quantum cosmology

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Abstract
Loop quantum cosmology allows for arbitrary superpositions of the triad variable. We show here how these superpositions can become indistinguishable from a classical mixture by the interaction with fermions. We calculate the reduced density matrix for a locally rotationally symmetric Bianchi I model and show that the purity factor for the triads decreases by decoherence. In this way, the universe assumes a definite orientation.

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1. Introduction

Quantum theory seems to be a universal framework for all interactions. As such, it should be applicable to the universe as a whole, leading to quantum cosmology. Since gravity is the dominant interaction on large scales, the formalism of quantum cosmology must be based on a theory of quantum gravity.

A direct quantization of general relativity in the canonical formalism leads to quantum geometrodynamics and the Wheeler–DeWitt equation [1]. An alternative canonical approach is loop quantum gravity [1, 2], which leads to loop quantum cosmology when applied to cosmological models [3, 4]. In loop quantum cosmology, the quantum state obeys a difference equation and not a differential equation. The reason for this is the presence of discrete spectra for geometric operators (such as the area operator) in the full theory. This discreteness seems to facilitate the avoidance of the classical big-bang singularity. Singularity avoidance thus seems to be more generic than in Wheeler–DeWitt quantum cosmology, although in the latter there exist models where the classical singularities are avoided, too [5].

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In loop quantum cosmology, one does not work with three-dimensional metrics, but with triads. This leads to an important difference to quantum geometrodynamics: triads can have two different orientations (left-handed and right-handed), which both lead to the same metric. A central question then concerns the role of the two orientations in the quantum theory. It has been claimed, for example, that the orientation of the triad reverses in a big-bang transition where the universe turns it inside out ([3], p 67). This assumes that the universe is always in a state of definite orientation. But because of its linear structure, quantum cosmology allows the occurrence of arbitrary superpositions of the two orientations; one would then expect that the universe is unlikely to be found in a definite orientation and that it is meaningless to talk about a change of orientation. How can this be understood?

This situation reminds one of an old problem for chiral molecules posed by Hund in the 1920s [6]. Many molecules occur as objects with a definite shape, although the underlying Hamiltonian is parity-invariant. Energy eigenstates, which are superpositions of chiral states, are typically found only for small molecules, such as ammonia, but not for bigger molecules such as sugar. The reason for the occurrence of chiral states as robust quantities was understood in the last decades and can be traced back to the process of decoherence—the irreversible emergence of classical properties by the unavoidable interaction with the environment [7, 8]. The spatial orientation of molecules is fixed by the scattering with photons and air molecules; the information about the superposition between different chiral states is transferred into the entanglement between the chiral molecules and the photons or air molecules and is no longer accessible at the molecules themselves.

In this paper, we shall examine whether decoherence is also responsible for the appearance of definite triad orientations in loop quantum cosmology. For this purpose, we need degrees of freedom that may serve as an appropriate ‘environment’ for the triads, in analogy with the photons or air molecules for the chiral molecules. Such an environment must be of fermionic nature, because bosonic variables only interact with the metric and are unable to discriminate between the two different orientations of a triad. (We assume here that there is no parity violation in the matter coupling.)

One possibility of implementing fermions into quantum cosmology is to consider inhomogeneous fermionic fluctuations superimposed on a homogeneous background [9]. In fact, decoherence by fermions in quantum cosmology was discussed at length some time ago [10, 11]. It was found there that a fermionic environment leads to a suppression of interferences for the scale factor and a background scalar field and thus to their classical appearance, but in a way that is less efficient than for a bosonic environment; the reason for this smaller efficiency can be traced back to the Pauli principle. Inhomogeneous (bosonic) fluctuations can, of course, become themselves relevant as a quantum system subject to decoherence. This is the case for the primordial fluctuations in inflationary cosmology, which can serve as the seeds for the origin of structure in the universe; their decoherence is discussed in [12] and other papers.

Here, we shall follow another route. Instead of taking inhomogeneous fermionic fluctuations, we retain homogeneity, but relax isotropy. Homogeneity demands any fields, including fermions, to be spatially constant. Imposing, in addition, isotropy would have the consequence that for fermions this constant is zero, because otherwise one could construct from the spinor fields a non-zero vector with a given direction, in contradiction to isotropy [13]. We therefore consider one of the simplest possible anisotropic models—the Bianchi I model (see, for example, [14] for a general introduction into classical and quantum aspects for such models). It is, in fact, the fermionic currents that in the considered model lead to the anisotropies. To simplify matters, we reduce this model further by imposing a rotational symmetry with respect to one axis, that is, by introducing the additional isotropy group U(1); one then arrives at a locally rotationally symmetric (LRS) model in which two of the diagonal
components of the connection and the triad are equal. This was also done in [13]. The fermionic current aligned in the one-direction of internal space is then the sole reason for the anisotropy. This model is admittedly very simple. We do, however, not expect that any of the qualitative features discussed here will change when going to more complicated models (such as the Gowdy model), although the technical difficulties will considerably increase.

The environment for the triads in the sense of decoherence is thus a homogeneous fermion field. It is known from quantum mechanics that one does not necessarily need many degrees of freedom for decoherence. For example, one can obtain decoherence from a long-range (e.g. gravitational) interaction between two bodies, where one body decoheres the other ([15], p 228).

In this paper, we shall basically use the model presented in [13] (fermions in a LRS Bianchi I model) and integrate over the fermions to study their decohering influence on the triads. But in order to investigate decoherence as a dynamical process, we have to introduce some notion of time. Quantum gravity is fundamentally timeless in the sense that there is no external time parameter present [1]. We thus introduce an inner variable and choose a massless scalar field $\varphi$ for this purpose. Such a field was used as an inner time in loop quantum cosmology for the Friedmann case in [16] and for the Bianchi I case (without fermions) in [17].

Section 2 contains a brief review of the formalism. Section 3 is the main part of our paper. We calculate the reduced density matrix and the linear entropy by tracing out the fermions and discuss the resulting decoherence. Section 4 contains our conclusions.

2. The formal framework

The formal framework of our discussion is based on the model of [13] supplemented by a massless scalar field. For the general formalism of fermions in loop quantum gravity, we refer to [18] and the references therein. As for the units, we set $c = 1$ but keep $G$ and $\hbar$ (although $G$ will not appear explicitly in (7) below).

In loop quantum gravity, the fundamental variables are constructed from the Ashtekar–Barbero connection $A^a_i(x)$ and the triad field $E^a_i(x)$ [1, 3]. Here, $i = 1, 2, 3$ is the internal index of the $su(2)$ algebra and $a = 1, 2, 3$ is the usual space index. The fundamental variables are fluxes (integrals of the $E^a_i(x)$ over two-dimensional surfaces) and holonomies (integrals of the $A^a_i(x)$ along curves). For Friedmann–Lemaître cosmology, the connection and the triad reduce to $A^a_i = c \delta^a_i$ and $E^a_i = p \delta^a_i$, respectively, where $|p| = a^2$ ($a$ is the scale factor) and $c$ is at the classical level given by $c = \gamma a$, where $\gamma$ denotes the Barbero–Immirzi parameter.$^1$

In the Bianchi I model, we have three scale factors instead of one. Therefore, instead of $c$ we have three variables called $\tilde{c}_1$, $\tilde{c}_2$ and $\tilde{c}_3$ (we use here tildes to follow the convention of [13]); instead of $p$, we have $p^1$, $p^2$ and $p^3$. In the LRS Bianchi I model used here, we have $\tilde{c}_2 = \tilde{c}_3$ and $p^2 = p^3$.

The fermions are described by a densitized current $\mathcal{J}_\alpha$, $\alpha = 0, 1, 2, 3$; we assume here, for simplicity, that $\mathcal{J}_2 = \mathcal{J}_3 = 0$. The fermionic current is a source of torsion, which leads to a new variable denoted below by $\phi$; this variable is, however, not a physical degree of freedom and can be connected to the fermionic current by the Gauss constraint. The fermionic current depends on the four half-densitized Grassmann variables $\Theta_1$, $\Theta_2$, $\Theta_3$ and $\Theta_4$ (summarized below under the label $\Theta$). In the quantum theory, one has for the non-vanishing components of the fermionic current operator the expressions

$$\mathcal{J}_0 = \hat{\partial}_\Theta \Theta_1 + \hat{\partial}_\Theta \Theta_2 - \hat{\partial}_\Theta \Theta_3 - \hat{\partial}_\Theta \Theta_4$$

$^1$ The Barbero–Immirzi parameter is called $\beta$ in [1], but we stick here to the convention of [13].
and
\[ \hat{J}_i/h = \partial_{\Theta_i} \Theta_1 + \partial_{\Theta_i} \Theta_2 + \partial_{\Theta_i} \Theta_3 + \partial_{\Theta_i} \Theta_4. \] (2)
In addition to the variables employed in [13], we introduce here a massless scalar field, which serves as an inner time variable. The classical Hamiltonian for it reads
\[ H_p = 8\pi G p^2 \left( \sqrt{|p^1| |p^2|} \right)^{-1}. \] (3)
(Because this Hamiltonian depends only on the absolute values of $p^1$ and $p^2$, one recognizes that it is insensitive to the triad orientation; this is why non-fermionic fields are not suitable to serve as a decohering environment.) For its quantization, we use the same technique as in [13]. The action of $\hat{p}_\phi$ on a state is given by $-ih\partial/\Theta_1\phi$.

Since one of the fundamental variables in loop quantum gravity is the holonomy, the connection has to be exponentiated also in loop quantum cosmology in order to arrive at mathematically well-defined expressions. (In homogeneous situations, the densitized triad components can be directly promoted to operators.) Functions on configuration space can then be expanded as follows:
\[ g(c_1, c_2, \phi) = \sum_{\mu_1, \mu_2, k} \xi_{\mu_1, \mu_2, k} \exp \left( \frac{i}{2} \mu_1 c_1 + \frac{i}{2} \mu_2 c_2 + ik\phi \right), \] (4)
where the sum is over finitely many $\mu_1, \mu_2 \in \mathbb{R}$ and $k \in \mathbb{Z}$. By solving the Gauss constraint for $p_\phi$ (the variable conjugate to $\phi$), we arrive, as in [13], at the difference equation (7) below, in which $k$ is eliminated. Therefore, we drop $k$ in the following.

A general state $|s\rangle$ is defined in the full Hilbert space $\mathcal{H} = \mathcal{H}_{\text{grav}} \otimes \mathcal{H}_{\text{fermion}} \otimes \mathcal{H}_\phi$ and can be expanded as follows:
\[ |s\rangle = \sum_{\mu_1, \mu_2} s(\mu_1, \mu_2, \Theta, \phi)|\mu_1, \mu_2\rangle, \] (5)
where the $|\mu_1, \mu_2\rangle$ denote the common eigenstates of the triad operators $\hat{p}^1$ and $\hat{p}^2$. Since $\mu_2 \rightarrow -\mu_2$ corresponds to a triad rotation, we demand
\[ s(\mu_1, \mu_2, \Theta, \phi) = s(\mu_1, -\mu_2, \Theta, \phi). \] (6)
In contrast to $\mu_2$, the sign of $\mu_1$ determines the relative orientation of the triad.

For the symmetric factor ordering, the difference equation for the total quantum state including the massless scalar field then reads
\[ \hat{h}s(\mu_1, \mu_2, \Theta, \phi) := 2((|\mu_2 + 3\delta_2| - |\mu_2 + \delta_2|)\sqrt{|\mu_1 + 2\delta_1|} + (|\mu_2 + \delta_2| - |\mu_2 - \delta_2|)\sqrt{|\mu_1 - 2\delta_1|} - 2(|\mu_2 + 3\delta_2| - |\mu_2 + 2\delta_2|)\sqrt{|\mu_1 - 2\delta_1|} + (|\mu_2 + 2\delta_2| - |\mu_2 - 2\delta_2|)\sqrt{|\mu_1 - 2\delta_1|})s(\mu_1 - 2\delta_1, \mu_2 + 2\delta_2, \Theta, \phi) - 2((|\mu_2 - 3\delta_2| - |\mu_2 - 2\delta_2|)\sqrt{|\mu_1 + 2\delta_1|} + (|\mu_2 + 2\delta_2| - |\mu_2 - 2\delta_2|)\sqrt{|\mu_1 + 2\delta_1|} - 2(|\mu_2 - 3\delta_2| - |\mu_2 - 2\delta_2|)\sqrt{|\mu_1 + 2\delta_1|} + (|\mu_2 + 3\delta_2| - |\mu_2 + 2\delta_2|)\sqrt{|\mu_1 - 2\delta_1|})s(\mu_1 + 2\delta_1, \mu_2 - 2\delta_2, \Theta, \phi) + (\sqrt{|\mu_1 + \delta_1|} - \sqrt{|\mu_1 - \delta_1|}) \cdot [(|\mu_2 + 2\delta_2|)s(\mu_1, \mu_2 + 2\delta_2, \Theta, \phi) - 4|\mu_2|s(\mu_1, \mu_2, \Theta, \phi) + (|\mu_2 + 2\delta_2|)s(\mu_1 + 2\delta_1, \mu_2 - 2\delta_2, \Theta, \phi) \{s(\mu_2 + 3\delta_2, \Theta, \phi) - s(\mu_2 + 2\delta_2, \Theta, \phi)\}] \] (7)
\[ \text{for simplicity, we choose } \alpha \rightarrow \infty \text{ for the non-minimal coupling parameter } \alpha \text{ in [13], which also leads to } \theta = 1 \text{ and } \beta = \gamma \text{ for the parameters } \theta \text{ and } \beta \text{ occurring in [13]. This has no qualitative influence on our results.} \]
In the following, we shall make the simplifications

\[ \text{Decoherence of triad orientations} \]

We shall now discuss how superpositions of different triad orientations can be suppressed by the interaction with fermions. We can then make the following ansatz for the solution:

\[
\rho_{\text{tot}} = \hat{s}(\mu_1', \mu_2', \Theta', \varphi) s(\mu_1, \mu_2, \Theta, \varphi).
\]

The increments \( \delta_1 \) and \( \delta_2 \) appearing in this difference equation arise from the edge lengths of spin networks in the full theory; in minisuperspace, their exact form and meaning remains open.

The gravitational constant \( G \) does not appear explicitly here because it has been absorbed in the process of expressing the inverse volume in terms of Poisson brackets [13].

We can write the difference equation (7) in the form

\[
\hat{hs}(\mu_1, \mu_2, \Theta, \varphi) = \frac{27T}{4} \left( c_1 \hat{J}_{1}^2 \hbar^2 + c_0 \hat{J}_{0}^2 \hbar^2 + c_\varphi \hat{P}_\varphi^2 \hbar^2 \right) s(\mu_1, \mu_2, \Theta, \varphi),
\]

where we have introduced

\[
T := |\mu_1|^{1/3} |\mu_2|^{1/3} (|\mu_1 + \delta_1|^{1/6} - |\mu_1 - \delta_1|^{1/6}) (|\mu_2 + \delta_2|^{1/3} - |\mu_2 - \delta_2|^{1/3})^2
\]

and

\[
c_1 := -\frac{\gamma^2}{1 + \gamma^2}, \quad c_0 := \frac{3\gamma^2}{1 + \gamma^2}, \quad c_\varphi := -16.
\]

We shall now discuss how superpositions of different triad orientations can be suppressed by the interaction with fermions.

### 3. Decoherence of triad orientations

In the following, we shall make the simplifications \( \Theta_2 = \Theta_3 = \Theta_4 = 0, \Theta_1 = \Theta \); we thus have \( \hat{J}_1^2 = 0 \) and \( \hat{J}_0^2 / \hbar^2 = \hat{J}_0 / \hbar = \partial_\Theta \Theta = 1 - \Theta \partial_\Theta \). The full equation (8) can then be written in the form

\[
\frac{27T}{4} c_0 \partial_\Theta \Theta s(\mu_1, \mu_2, \Theta, \varphi) = \hat{g} s(\mu_1, \mu_2, \Theta, \varphi),
\]

with

\[
\hat{g} := \hat{h} + \frac{27T}{4} \left( c_0 + c_\varphi \hat{P}_\varphi^2 \right).
\]

We can then make the following ansatz for the solution:

\[
s(\mu_1, \mu_2, \Theta, \varphi) = s_0(\mu_1, \mu_2, \varphi) + \Theta s_1(\mu_1, \mu_2, \varphi).
\]

From (11), one then obtains the following two equations:

\[
\hat{g} s_1(\mu_1, \mu_2, \varphi) = \frac{27T}{4} c_0 s_1(\mu_1, \mu_2, \varphi),
\]

\[
\hat{g} \delta_0(\mu_1, \mu_2, \varphi) = 0.
\]

Since the total system is in a pure state, the total density matrix reads

\[
\rho_{\text{tot}} = \hat{s}(\mu_1', \mu_2', \Theta', \varphi) s(\mu_1, \mu_2, \Theta, \varphi).
\]
Using the rules for Grassmann integration (see e.g. [19]), one can define the following reduced density matrix for the gravitational variables alone:

\[ \rho_{\text{red}}(\mu_1, \mu_2; \mu_1', \mu_2'; \varphi) = \int d\Theta d\bar{\Theta} e^{-\Theta \bar{\Theta}} \bar{s}(\mu_1', \mu_2', \Theta, \varphi) s(\mu_1, \mu_2, \Theta, \varphi). \]  

(17)

The integration yields

\[ \rho_{\text{red}}(\mu_1, \mu_2; \mu_1', \mu_2'; \varphi) = \bar{s}_1(\mu_1', \mu_2', \varphi)s_1(\mu_1, \mu_2, \varphi) + \bar{s}_0(\mu_1', \mu_2', \varphi)s_0(\mu_1, \mu_2, \varphi). \]  

(18)

The total density matrix corresponds to an entangled state if both terms are present in expression (18) for the reduced density matrix, that is, if both \( s_0 \) and \( s_1 \) are non-vanishing. Otherwise, the gravitational part is by itself in a pure state and there is no decoherence. This is also obvious from (13).

A measure for the purity of the total state (16) is the trace of \( \rho_{\text{red}}^* \rho_{\text{red}} \), which is equal to 1 for a pure state and smaller than 1 for a mixed state; it is directly related to the linear entropy

\[ S_{\text{lin}} = 1 - \text{tr} \rho_{\text{red}}^2 \]  

[7]. One could also address the von Neumann entropy \(-k_B \text{tr} (\rho_{\text{red}} \ln \rho_{\text{red}})\), but for the present purpose it is sufficient to restrict to \( S_{\text{lin}} \).

To obtain concrete results, we calculate the evolution of the coefficients \( s_0 \) and \( s_1 \) in (15). The spatial parameters \( \mu_1 \) and \( \mu_2 \) span a two-dimensional discrete lattice on which we have to choose appropriate initial data. Solving the equations in (15) for the derivative in the continuous variable \( \varphi \), we have

\[ \partial^2_{\varphi}s_1 = -\frac{1}{108} \hat{h}s_1, \]  

(19)

\[ \partial^2_{\varphi}s_0 = -\frac{1}{108} \hat{h}s_0 - \frac{3\gamma^2}{16(1 + \gamma^2)} s_0. \]  

(20)

Here, \( \hat{h}s \) denotes the gravitational part of the difference equation, as given by the left-hand side of (7).

To deal with (20), which is a combination of difference and differential equations, we use standard numerical techniques, implemented in a C source code written by ourselves. For this purpose, we have to discretize the continuous variable \( \varphi \). Since the equations in (20) are of second order in \( \varphi \), we decompose them into a system of first-order equations. The resulting equations can be solved, for example, with the fourth-order Runge–Kutta algorithm [20]. Now, we are in a position to calculate the coefficients \( s_0 \) and \( s_1 \) numerically, from which we then obtain immediately the functions \( s \) in the expansion of the state (5). Our computer code can be found on the link given in [21].

We now briefly describe the steps for the calculation of the reduced density matrix. As initial data at \( \varphi = 0 \) we have to specify \( s_0 \), \( s_1 \) and their derivatives. We choose them to be Gaussians, normalized by the condition \( \text{tr} \rho_{\text{red}} = 1 \), except for \( s_1(\varphi = 0) \), which is set equal to zero. This provides us with an unentangled state in the beginning of the evolution, see (18). Since \( s_1 \) vanishes initially, but not its derivative, the state will evolve into a mixed state. In the long-term evolution, it turns out that \( s_1 \) will dominate over \( s_0 \) and the state will be pure again, as only the first term in (18) is left; this, however, happens for times much longer than the times for which the model is applicable.

The iteration at each time step starts with the calculation of \( s_0 \) and \( s_1 \), as described above. The evolution preserves the normalization \( \text{tr} \rho_{\text{red}} = 1 \) for the reduced density matrix; small deviations from this condition, which occur due to numerical errors, are corrected in each time step. Since the initial state is unentangled, \( \text{tr} \rho_{\text{red}}^2 \) is initially equal to 1. As the inner time variable increases, the total state becomes entangled, and the purity factor decreases—the gravitational variables are in a mixed state, and decoherence becomes more and more efficient. The result can be plotted as a function of the inner time variable \( \varphi \), see figure 1.
Figure 1. The purity factor $\text{tr}\rho^2$ plotted against the inner time variable $\phi$.

The interesting region is the right half of the diagram, where the purity factor decreases rapidly. In our simulation, the step size $\delta_1$ resp. $\delta_2$ is chosen in such a way that it is large in the beginning and smaller in the area of interest. As a test of the numerical robustness, we checked the algorithm with different numerical step sizes and different initial data. As long as the data are chosen as described above, the resulting curves look very similar. Another test is to choose the simpler Euler algorithm instead of the Runge–Kutta procedure. The qualitative behaviour is the same for both procedures.

For the calculation, we have to fix the Barbero–Immirzi parameter $\gamma$ in (7). In principle, $\gamma$ is a free parameter leading to a one-parameter ambiguity in the quantization. In most simulations, we have chosen $\gamma = 0.238$, which is motivated by the desire to obtain the correct Bekenstein–Hawking entropy for black holes [22]. However, we have found that our results are largely independent of the specific choice for $\gamma$.

4. Conclusion

In summary, one can say that fermions ‘measure’ the orientation of the triad in loop quantum cosmology. In this sense, they provide the universe with a definite orientation. The fermions act as an environment similarly to the photons or air molecules that can provide molecules with a definite shape. Fermions are thus an important ingredient in loop quantum cosmology.

If the orientation is fixed by decoherence, then it is hard to imagine a scenario in which the universe changes orientation by going from a pre- to a post-big-bang scenario. One only has different branches of the total quantum state with different orientations. These branches are independent of each other, except possibly for small universes in which the decohering influence can be neglected, similarly to small molecules such as ammonia for which the influence of the environment is too weak to suppress the interferences between different chiral states. But in this case we expect that the universe is in a superposition of left and right
orientations and that there is no meaning of a classical transition between the two orientations; a permanent tunnelling then occurs, similar to the ammonia molecule.

The situation may be compared to a scenario discussed in string quantum cosmology some time ago [23]. In a semiclassical picture, the standard big bang is preceded in time (perhaps through a singularity) by a pre-big-bang state. However, a consistent analysis in the quantum theory shows that wave packets cannot be continued through the singularity and that pre- and post-big-bang just correspond to independent components of the total wave function that decohere from each other. Another example in quantum cosmology is the decoherence of the ‘cosmological constant’ (dark energy) by the interaction with metric perturbations [24].

To facilitate the discussion of decoherence as a process in time, we have introduced a massless scalar field $\phi$ to serve as an intrinsic time parameter. This, however, implicitly assumes that $\phi$ is already a decohered variable. Its decoherence can emerge, for example, by the interaction with inhomogeneous perturbations as discussed in [10]. But, again, one would not expect this decoherence to be efficient for small universes. For this situation, one would be left with a timeless quantum state for which the traditional concept of evolution breaks down.

The increase of entropy (decrease of the purity factor) arises because a special initial state is chosen. This initial state is characterized by the absence of entanglement between the gravitational and fermionic degrees of freedom. An initial unentangled state may be at the heart of the origin of irreversibility in our Universe [25, 26]. How this origin can be understood in full loop quantum cosmology is left for future investigations.

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