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## Generalized uncertainty principles and localization of a particle in discrete space

Martin Bojowald and Achim Kempf
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# Generalized uncertainty principles and localization of a particle in discrete space 

Martin Bojowald<br>Institute for Gravitation and the Cosmos, The Pennsylvania State University, 104 Davey Lab, University Park, PA 16802<br>Achim Kempf<br>Department of Applied Mathematics, University of Waterloo, Waterloo, Ontario, N2L 3G1, Canada


#### Abstract

Generalized uncertainty principles are able to serve as useful descriptions of some of the phenomenology of quantum gravity effects, providing an intuitive grasp on non-trivial space-time structures such as a fundamental discreteness of space, a universal bandlimit or an irreducible extendedness of elementary particles. In this article, uncertainty relations for single-particle quantum mechanics are derived by a moment expansion of states for quantum systems with a discrete coordinate, and correspondingly a periodic momentum. Corrections to standard uncertainty relations are found, with some similarities but also key differences to what is often assumed in this context. The relations provided can be applied to discrete models of matter or space-time, including loop quantum cosmology.


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## I. INTRODUCTION

If space is discrete, the form of its underlying structure should influence the general properties of position and momentum measurements and therefore their fundamental uncertainty relations. In this context, see e.g., [1]-[5]. Compared with standard quantum mechanics, there may be additional limitations to the precision of measurements, as they can often be captured in generalized uncertainty principles, see e.g., [6]-[10]. For general reviews, see e.g. [11],[12]. Phenomenology and experimental proposals are discussed, e.g., in [13]-[17].

Modifications to the uncertainty principle are bound to arise because the momentum, on a discrete space, is no longer defined in all situations; in general, it must be replaced by finite translation operators for displacements of at least the lattice spacing. For studies on the question of momentum conservation in this context, and varying minimum uncertainties, see, e.g., [18]-[23].

On scales larger than the lattice spacing, one may introduce an approximate momentum operator, just as one can define approximate plane waves of wavelength larger than the spacing. However, as the wave length approaches the discreteness scale, the underlying structure becomes noticeable and deviations from standard properties of momentum arise.

In the context of the low-energy regime of various approaches to quantum gravity it is therefore of interest to explore the consequences of spatial discreteness for the basic uncertainty relations. In this paper, we present a systematic method to compute the leading corrections to the position and momentum uncertainty relations for discrete spaces. Differences to some common assumptions about such principles are pointed out. We begin this article with a brief review of the mathematical structures involved in discrete matter systems on the one hand, and some approaches to quantum gravity on the other. Our discussion will focus on localization, in the sense of minimizing fluctuations in position, and we will study uncertainty principles without needing to refer to specific representations. In the main part of this article, Section III, we will then systematically derive the generalized uncertainty principle for a discrete system.

## II. SPATIAL DISCRETENESS

There are numerous examples of discrete structures in physical models, such as crystals that have periodic potentials. As an illustration, let us consider the 1-dimensional quantum mechanical system of Bloch states. For wavelike excitations of a length well above the periodicity of the crystal, one may start with free scattering states $\exp (i k q)$ in the position representation, whose energy is $E(k)=\hbar^{2} k^{2} / 2 m$ if they represent particles of mass $m$. These states are no longer energy eigenstates if the particles move in a non-trivial periodic potential $V(q)$ with $V\left(q+q_{0}\right)=V(q)$, where $q_{0}$ is the periodicity. We decompose the set of plane waves into sectors labeled by a real number $\epsilon \in[0,2 \pi)$ in one-to-one correspondence with wave functions on the finite interval $\left[0, q_{0}\right]$ subject to the "almost periodic" boundary condition $\psi\left(q+q_{0}\right)=e^{i \epsilon} \psi(q)$. Square integrable functions satisfying these boundary conditions define the Hilbert spaces $\mathcal{H}_{\epsilon}$. Parameterized by $\epsilon$ for all the sectors, momentum eigenstates are then

$$
\begin{equation*}
\psi_{n}^{(\epsilon)}(q)=\exp \left(i \mu_{n}^{(\epsilon)} q\right) \tag{1}
\end{equation*}
$$

where for all integers $n$,

$$
\begin{equation*}
\mu_{n}^{(\epsilon)}:=\frac{2 \pi n+\epsilon}{q_{0}} \tag{2}
\end{equation*}
$$

is proportional to the momentum eigenvalues

$$
\begin{equation*}
p_{n}^{(\epsilon)}=\hbar \mu_{n}^{(\epsilon)} . \tag{3}
\end{equation*}
$$

For each fixed $\epsilon$, these are the discrete momentum eigenvalues of a particle on a circle with $e^{i \epsilon}$-periodicity, and together, for all $\epsilon$, they fill the whole real line. In this heuristic way, the continuous momentum spectrum for a particle in the periodic potential is recovered. This statement is heuristic because the Hilbert spaces $\mathcal{H}_{\epsilon}$ are all different as function spaces and independent for different $\epsilon$, and a wave function $\psi_{n}^{(\epsilon)}(q)$ would not be normalizable in the usual continuum Hilbert space $L^{2}(\mathbb{R}, \mathrm{~d} q)$. One may view the Hilbert spaces of different $\epsilon$ as superselection sectors in the direct sum $\bigoplus_{\epsilon} \mathcal{H}_{\epsilon}$ : One would consider all states as lying in the same Hilbert space, but allow superpositions only of states within the same $\mathcal{H}_{\epsilon}$. (The full direct-sum Hilbert space is non-separable.)

In contrast to the momentum spectrum, the energy spectrum in a given periodic potential $V(q)$, while continuous, need not fill the whole real line. By solving the energy eigenvalue equation for each $\epsilon, \hat{H} \psi_{k}^{(\epsilon)}=E^{(\epsilon)}(k) \psi_{k}^{(\epsilon)}$ where $\psi_{k}^{(\epsilon)}$ is subject to the almost-periodicity
condition, one obtains a function $E^{(\epsilon)}(k)$. Combining all values for the different $\epsilon$ in general leaves out some real numbers which are not realized as an energy eigenvalue in the periodic potential, and the band structure of excitation spectra emerges.

Functional analytically, the differential operator $-\hbar^{2} \partial_{q}^{2} / 2 m+V(q)$, when considered on the finite interval of one periodicity length, becomes self-adjoint once suitable boundary conditions are imposed. Its spectrum depends on the boundary conditions. The operator has deficiency indices $(2,2)$ and thus possesses a family of self-adjoint extensions parameterized by $\mathrm{U}(2)$. Our previous boundary conditions $\psi\left(q+q_{0}\right)=\psi(q) e^{i \epsilon}$ combined with $\psi^{\prime}\left(q+q_{0}\right)=$ $\psi^{\prime}(q) e^{i \epsilon}$ amount to a subgroup $\mathrm{U}(1) \subset \mathrm{U}(2)$. For each choice of such a boundary condition, i.e, for each choice of $\epsilon \in[0,2 \pi)$, we obtain a different self-adjoint extension $\hat{H}_{\epsilon}$, each possessing its own spectrum and eigenvectors. Each set of eigenvectors spans the same Hilbert space of square integrable functions over the interval, and the union of these spectra forms the bands.

Clearly, the underlying periodicity of the crystal, by leading to the band structure, has direct implications for the dynamics, which allows one to probe underlying properties of $V(q)$ in experiments. In low-energy experiments, distance scales larger than the spatial periodicity can easily be probed and described perturbatively, for instance by corrected dispersion relations taking into account the microstructure. Of interest in the present context is the fact that a discrete structure arises in momentum space as a consequence of periodicity in position space.

Some approaches to quantum cosmology, especially loop quantum cosmology [24, 25] (see [26] for a recent review), begin with a similar but reversed setting, now dealing with discrete space and almost periodic or compactified momentum space. In this case, space is not represented by position coordinates but by geometrical quantities such as the total volume $V$ of an isotropic universe model, or in general by points in minisuperspace. The momentum $P$ is then related to curvature components or, in cosmology, the Hubble parameter. As with Bloch states, the Hilbert space (in the momentum representation) is spanned by states

$$
\begin{equation*}
\psi_{n}^{(\epsilon)}(P)=\exp \left(i \mu_{n}^{(\epsilon)} P\right) \tag{4}
\end{equation*}
$$

with the same form (2) of $\mu_{n}^{(\epsilon)}$ as before, except that $q_{0}$ is to be replaced by a quantity $P_{0}$ signaling the periodicity of $P[27,28] .[65]$ These are the main aspects of loop quantum cosmology we need in this article; see Appendix A for more details.

In addition to technical properties of the dynamics, there is a key physical difference between the treatment of Bloch waves as a model for condensed matter physics and isotropic loop quantum cosmology as a model for quantum gravity: Bloch states represent a system in which the position coordinate $q$ is almost periodic, and thus its momentum is discrete. The regime of distances $q \gg q_{0}$ much larger than the periodicity is easily accessible by classical physics, and one is interested in uncovering what happens at smaller distances near the scale of periodicity. In loop quantum cosmology, on the other hand, the (momentum-like) expansion rate $P$ is almost periodic while the size $V$ is discrete. Moreover, it is the lowcurvature regime $P \ll P_{0}$ which is easily accessible by classical physics and one is interested in uncovering what happens at large curvature near $P_{0}$. This point plays an important role regarding the specific questions one tries to address. In this article, we will mainly be concerned with the quantum-cosmology-like situation, probing the quantum system well below the periodicity scale. This regime will be implemented by the approximations used.

## A. Uncertainty with periodic momenta

Motivated by the examples of discrete systems, we assume a general class of models with a periodicity condition on the momentum: wave functions $\phi(p)$ in momentum space obey $\phi\left(-p_{0} / 2\right)=\phi\left(p_{0} / 2\right)$ for some momentum value $p_{0}$. Compared to the more general discussion before, we set $\epsilon=0$ without loss of generality; non-zero values will simply shift the lattice structure we obtain in position space. Here, the superselection assumption is important. The conjugate variable $q$ is then quantized to an operator with discrete spectrum $q_{n}=2 \pi \hbar n / p_{0}$ with integer $n$. We will analyze the possible values of uncertainties that can be realized in the set $\mathcal{F}_{\bar{q}}$ of wave functions that possess some fixed position expectation value $\bar{q}=\langle\hat{q}\rangle$. In particular, we ask how small the position fluctuation $\Delta q$ can be in this set, or how well we can localize a particle at position $\bar{q}$. Our aim is to derive a function $\Delta q_{\text {min }}(\bar{q})$ which determines the minimally possible uncertainty for localization at $\bar{q}$.

If we choose $\bar{q}$ to be one of the lattice points, $q_{n}$, we may localize the particle arbitrarily sharply because we could choose the state to be the $\hat{q}$-eigenstate with eigenvalue $q_{n}$. Thus, $\Delta q_{\min }\left(q_{n}\right)=0$. As we will show now, for all other values of $\bar{q}$ the minimum uncertainty is not zero.

Without loss of generality, we then choose $q_{0}=0<\bar{q}<q_{1}=2 \pi \hbar / p_{0}$. A corresponding
wave function can no longer be a position eigenstate, and in order to achieve minimum position uncertainty we should choose a superposition of the eigenstates with position eigenvalue zero and $q_{1}$ :

$$
\phi_{\bar{q}}(p)=a e^{-i q_{0} p}+b e^{-i q_{1} p}=a+b e^{-2 \pi i p / p_{0}} .
$$

With normalization, $|a|^{2}+|b|^{2}=1 / p_{0}$. Moreover, we straightforwardly compute

$$
\begin{equation*}
\bar{q}=2 \pi \hbar|b|^{2} \quad, \quad\left\langle\hat{q}^{2}\right\rangle=4 \pi^{2} \hbar^{2}|b|^{2} / p_{0} \tag{5}
\end{equation*}
$$

Eliminating $|b|$, we obtain

$$
\begin{equation*}
\Delta q_{\min }(\bar{q})=\sqrt{\bar{q}\left(q_{1}-\bar{q}\right)} \quad \text { for } \quad 0 \leq \bar{q} \leq q_{1} \tag{6}
\end{equation*}
$$

extended periodically over the whole $q$-axis, consistent with the findings in [22]. For sectors with $\epsilon \neq 0$, we obtain the same formula just with $q_{1}$ interpreted as the lattice spacing $L=q_{1+\epsilon}-q_{\epsilon}=q_{1}$. The minimal uncertainty indeed vanishes for $\bar{q}$ a lattice point, and is at most half the lattice spacing: $\Delta q_{\min } \leq L / 2$. At this stage we see the importance of the superselection assumption. Without it, we could have made the minimal uncertainty arbitrarily small for all $\bar{q}$; for every $\bar{q}$, there is an $\epsilon$-sector containing a $\hat{q}$-eigenstate with eigenvalue $\bar{q}$. From the perspective of minimally possible position uncertainty, the discreteness is thus noticeable only if the $\epsilon$-sector is fixed, for instance derived from other observations. On one hand, if all $\epsilon$-sectors were allowed, we could localize at every point with absolute precision. On the other hand, if instead in momentum space the boundary condition of periodicity up to a phase $e^{i \epsilon}$ is replaced by Dirichlet boundary conditions then $\hat{p}$ is symmetric but it is not self-adjoint. In this case, at no point could the position be resolved to absolute precision, leading to a global finite $\Delta q_{\text {min }}$. We will also encounter this case below.

We now turn to momentum uncertainties. The minimum position uncertainty can be used to probe the lattice structure only if the resolution of our measurements is close to the lattice spacing. Moreover, the $\epsilon$-sector would have to be determined by independent means. An important question then is how the lattice structure can be noticed if measurements are done at energies which may be high, but not high enough to resolve the lattice. One way that may offer an opportunity to overcome this problem may be to test for small deviations from the usual uncertainty relations, namely by checking the relationship between both position and momentum fluctuations. Before we enter a more detailed discussion of generalized
uncertainty relations, for later comparisons it will be useful to continue with the question of localization and compute some of the corresponding momentum uncertainties.

Again, we choose a position eigenstate of one of the lattice points, without loss of generality at $\bar{q}=q_{0}=0$. Then, $\phi_{q_{0}}(p)=1 / \sqrt{p_{0}}$. In addition to $\bar{q}=0$ and $\Delta q=0$, we have $\bar{p}=\langle\hat{p}\rangle=0$ and $\Delta p=p_{0} / 2 \sqrt{3}$. One of the consequences of discreteness is that $\Delta q=0$ is possible with finite $\Delta p$, clearly requiring modified uncertainty relations compared to the continuum case. It will also be useful to consider higher moments of the state, in particular

$$
\begin{equation*}
\Delta\left(p^{n}\right):=\left\langle(\hat{p}-\bar{p})^{n}\right\rangle=\frac{p_{0}^{n}}{2^{n}(n+1)} \tag{7}
\end{equation*}
$$

for even $n$ while $\Delta\left(p^{n}\right)=0$ if $n$ is odd. The series $\Delta\left(p^{n}\right) / p_{0}^{n}$ thus falls off for increasing $n$.

## B. Generalized uncertainty relations

As the preceding example demonstrates, quantum systems with discrete or periodic structures in phase space cannot obey the usual uncertainty relation $\Delta q \Delta p \geq \hbar / 2$ of quantum mechanics because the lattice structure makes it possible for $\Delta q$ to vanish at finite $\Delta p$. Nevertheless, we still expect some form of uncertainty relation to apply; after all, at distance scales much larger than the lattice spacing we should be able to recover standard continuum quantum mechanics. A common way to parameterize generalized uncertainty relations is

$$
\begin{equation*}
\Delta q \Delta p \geq \frac{\hbar}{2}\left(1+\alpha(\Delta p)^{2}+\beta(\Delta q)^{2}+\gamma\right) \tag{8}
\end{equation*}
$$

considered first in [6], see also, e.g., [8-10].
The parameters $\alpha, \beta$ and $\gamma$ are independent of $\Delta q$ and $\Delta p$ but in general may depend on expectation values of the overall state. Dimensional analysis of the correction terms in Eq. (8) indicates that these parameters are not purely quantum corrections, as perhaps motivated by quantum gravity. If one uses only Planck's constant and the Planck length, dimensionally we must have $\alpha \propto \ell_{\mathrm{P}}^{2} / \hbar^{2}=G / \hbar$ and $\beta \propto 1 / \ell_{\mathrm{P}}^{2}=1 / G \hbar$, both proportional to $\hbar^{-1}$. As quantum corrections, this behavior is unsuitable because the terms $G(\Delta p)^{2} / \hbar$ and $(\Delta q)^{2} / G \hbar$ do not necessarily go to zero for $\hbar \rightarrow 0$, with semiclassical fluctuations squared usually being about the size of $\hbar$. Generalized uncertainty principles thus require either modifications to the quantum algebra of basic operators and even the classical symplectic structure, or an additional scale not directly related to $\hbar$. This additional scale could be the
bandlimit of a fundmental bandlimitation [30], the size of fundamental extended objects, or the periodicity or discreteness scale considered in this paper.

## 1. Implications

In Eq. (8), let us first consider the case where $\alpha, \beta>0, \gamma>-1$. If also $\alpha \beta \geq 1 / \hbar^{2}$, then this uncertainty principle has no solutions, i.e., we can rule out this case: for $x:=\Delta q / \sqrt{\alpha} \hbar$ and $y:=\sqrt{\alpha} \Delta p$ the relation implies the impossible relationship $(x-y)^{2} \leq-(1+\gamma)<0$. Else, if $\alpha, \beta>0$ and $\alpha \beta \leq 1 / \hbar^{2}$, then the uncertainty relation (8) arises from the commutation relation

$$
\begin{equation*}
[\hat{q}, \hat{p}]=i \hbar\left(1+\alpha \hat{p}^{2}+\beta \hat{q}^{2}\right) \tag{9}
\end{equation*}
$$

through $\Delta A \Delta B \geq \frac{1}{2}|\langle[A, B]\rangle|$ which holds for any symmetric or self-adjoint operators $A, B$ on any domain on which they and their commutator can act. Notice that (9) induces an uncertainty relation of the type of (8) with a generally non-vanishing $\gamma$ that depends on $\langle\hat{q}\rangle$ and $\langle\hat{p}\rangle$. A Hilbert space representation can be constructed using $\rho$-deformed raising and lowering operators, $\hat{a}, \hat{a}^{\dagger}$. (In the literature on quantum groups, the parameter $\rho$ is usually denoted $q$, but we here use the symbol $q$ for the position operator). Namely, in this case the operators $\hat{q}$ and $\hat{p}$ can be represented through

$$
\begin{align*}
& \hat{q}:=\frac{1}{\sqrt{2 \beta(1 / \hbar \sqrt{\alpha \beta}-1)}}\left(\hat{a}^{\dagger}+\hat{a}\right)  \tag{10}\\
& \hat{p}:=\frac{i}{\sqrt{2 \alpha(1 / \hbar \sqrt{\alpha \beta}-1)}}\left(\hat{a}^{\dagger}-\hat{a}\right) \tag{11}
\end{align*}
$$

where $\hat{a}, \hat{a}^{\dagger}$ obey

$$
\begin{equation*}
\hat{a} \hat{a}^{\dagger}-\rho \hat{a}^{\dagger} \hat{a}=1 \tag{12}
\end{equation*}
$$

with

$$
\begin{equation*}
\rho:=\frac{1+\hbar \sqrt{\alpha \beta}}{1-\hbar \sqrt{\alpha \beta}} \tag{13}
\end{equation*}
$$

Note that $\rho \in(1, \infty)$. As usual, the Hilbert space together with a representation of $\hat{q}$ and $\hat{p}$ can be constructed by the Fock method on a state $|0\rangle$ obeying $\hat{a}|0\rangle=0$. For a general analysis of $q$-deformed $a-a^{\dagger}$ commutation relations, see also [31].

For $\beta=0$, the representations of the generalized commutation relation $[\hat{q}, \hat{p}]=i \hbar\left(1+\alpha \hat{p}^{2}\right)$ are discussed in [10], where it was found that their properties qualitatively depend on the $\operatorname{sign}$ of $\alpha$ :

- For $\alpha<0$, there are finite-dimensional representations. In infinite-dimensional ones, $\hat{p}$ is a bounded operator and has a finite range of eigenvalues; $\hat{q}$ possesses self-adjoint extensions whose spectra are continuous.
- For $\alpha>0, \hat{p}$ has a continuous spectrum comprised of the entire real line. The selfadjoint extensions of $\hat{q}$ possess discrete parts to their spectra and normalizable eigenvectors.

Let us now return to Eq. (8) for generic $\alpha, \beta$ and $\gamma$. It is of particular interest to probe the smallest allowed scales by determining how small $\Delta q$ can be made. In the case $\alpha>0$, $\beta>0, \gamma>-1, \alpha \beta \leq 1 / \hbar^{2}$ of above, it is known that $\Delta q$ possesses a non-vanishing minimum overall, as we will recover as a special case. But we also expect that, in other cases, the vanishing of $\Delta q$ may be possible for finite $\Delta p$ as required for lattice models.

We begin by noticing that saturating the uncertainty relation requires

$$
\begin{equation*}
\Delta q=\frac{\Delta p \pm \sqrt{\left(1-\hbar^{2} \alpha \beta\right)(\Delta p)^{2}-\hbar^{2} \beta(1+\gamma)}}{\hbar \beta} . \tag{14}
\end{equation*}
$$

For fixed $\alpha, \beta$ and $\gamma$ this expression is minimized for

$$
(\Delta p)^{2}=\frac{1+\gamma}{\alpha\left(1-\hbar^{2} \alpha \beta\right)}
$$

such that the uncertainty in position is bounded from below by

$$
\begin{equation*}
\Delta q=\hbar \sqrt{\frac{\alpha(1+\gamma)}{1-\hbar^{2} \alpha \beta}} \tag{15}
\end{equation*}
$$

provided the square root is well-defined. For $\alpha(1+\gamma)>0$ a positive lower bound for the position uncertainty results independently of the momentum uncertainty as in the example of Section II A in the case of Dirichlet boundary conditions. If instead $\alpha<0$ and $1+\gamma>0$, then the generalized uncertainty relation Eq. (8) allows $\Delta q$ to vanish at finite $\Delta p=\sqrt{-(1+\gamma) / \alpha}$, qualitatively similar to our example above when fixing an $\epsilon$-sector. This confirms our expectation that the coefficients in generalized uncertainty relations, and especially their signs, carry information about underlying discrete structures.

Indeed, even if no direct information is available about the boundary conditions in momentum space, such as the specific $\epsilon$-sector, indications of negative values of $\alpha$ (for positive $1+\gamma$ ) would imply agreement with the discrete model, while positive $\alpha$ would correspond to a finite lower bound to the position uncertainty (15).

## 2. Representations

Properties of operators and Hilbert-space representations can be surprisingly subtle in the context of generalized uncertainty relations. In order to illustrate this, let us have a closer look at the case of $\alpha, \beta>0$, i.e., at the case of a finite lower bound to the position uncertainty. The operators $\hat{q}$ and $\hat{p}$ then act via Eqs. (10), (11), on the domain, $D$, of all finite complex linear combinations of the basis vectors $\left(a^{\dagger}\right)^{n}|0\rangle$. Clearly, $D$ is dense in the Hilbert space, $\mathcal{H}$, of all (finite or infinite) normalizable linear combinations of the vectors $\left(a^{\dagger}\right)^{n}|0\rangle$. It is straightforward to verify that the commutation relation holds on $D$ and that $\hat{q}$ and $\hat{p}$ are symmetric operators, i.e., that all their expectation values are real: $\langle\phi| \hat{q}|\phi\rangle \in \mathbb{R}$ and $\langle\phi| \hat{q}|\phi\rangle \in \mathbb{R}$ for all $|\phi\rangle \in D$. As always in quantum mechanics, we obtain the physical domain $D_{\text {physical }}$ by enlarging $D$ so as to include as many infinite linear combinations of the basis vectors $\left(a^{\dagger}\right)^{n}|0\rangle$ as possible. Concretely, $D_{\text {physical }} \subset \mathcal{H}$ is the maximal domain on which the commutation relation holds. This means that $D_{\text {physical }}$ is the maximal domain on which the images of all operators that occur in the commutation relations are contained in the Hilbert space. Therefore, $D_{\text {physical }}$ is the set of all $|\phi\rangle \in \mathcal{H}$ for which $\hat{q}|\phi\rangle \in \mathcal{H}, \hat{p}|\phi\rangle \in \mathcal{H}$, $\hat{q} \hat{p}|\phi\rangle \in \mathcal{H}, \hat{p} \hat{q}|\phi\rangle \in \mathcal{H}, \hat{q}^{2}|\phi\rangle \in \mathcal{H}$ and $\hat{p}^{2}|\phi\rangle \in \mathcal{H}$.

In this context, let us recall that the presence of finite lower bounds to $\Delta q$ and $\Delta p$ precludes the existence of eigenvectors of $\hat{q}$ or $\hat{p}$ in $D_{\text {physical }}$ since they would have vanishing variance, $\Delta q=0$ or $\Delta p=0$. The lower bounds even preclude the existence of sequences of physical vectors whose variance, say $\Delta q$, goes to zero (even while allowing that $\Delta p$ might diverge). As one might expect, therefore, $\hat{q}$ and $\hat{p}$ on $D_{\text {physical }}$ have no complete spectral decomposition and therefore cannot be self-adjoint [6]. The phenomenon that operators, such as $\hat{q}$ and $\hat{p}$, are symmetric on a domain, here $D_{\text {physical }}$, without being self-adjoint, is a subtlety that can occur only in infinite-dimensional Hilbert spaces.

Interestingly, the detailed functional analysis of these operators shows that $\hat{q}$ and $\hat{p}$ individually do possess extensions of their domain on which they become self-adjoint. In particular, there exists a family of enlarged domains $D_{q, \alpha}$, parametrized by $\alpha \in[0,1)$, obey$\operatorname{ing} D_{\text {physical }} \subset D_{q, \alpha} \subset \mathcal{H}$ such that for each fixed $\alpha$ the extended $\hat{q}_{\alpha}$ which acts on $D_{q, \alpha}$ is self-adjoint and has a discrete spectrum, $\left\{q_{n, \alpha}\right\}_{n \in \mathbb{Z}}$, along with normalizable eigenvectors $\left\{\left|q_{n, \alpha}\right\rangle\right\}_{n \in \mathbb{Z}}$. It has been shown that as $\alpha$ runs through the interval $[0,1)$, the corresponding discrete grids of eigenvalues $\left\{q_{n, \alpha}\right\}$ cover the real line exactly once, $\bigcup_{\alpha \in[0,1)}\left\{q_{n, \alpha}\right\}_{n \in \mathbb{Z}}=\mathbb{R}$.

The fact that $\hat{q}_{\alpha}$ possesses eigenvectors $\left\{\left|q_{n, \alpha}\right\rangle\right\}_{n \in \mathbb{Z}}$, for which $\Delta q_{\alpha}=0$, is consistent with the fact that we have a positive lower bound (15) for $\Delta q$. The reason is of course that the eigenvectors $\left|q_{n, \alpha}\right\rangle$ are in $D_{q, \alpha}$ but not in $D_{\text {physical }}$.

Nevertheless, while keeping in mind that the vectors $\left|q_{n, \alpha}\right\rangle$ are not in the physical domain, we may of course utilize the fact that any such set of eigenvectors, $\left\{\left|q_{n, \alpha}\right\rangle\right\}_{n \in \mathbb{Z}}$, for any fixed $\alpha$, is a basis in the Hilbert space. Namely, we can use the fact that any physical state $|\phi\rangle \in D_{\text {physical }}$ is completely specified by its coefficients $\left\langle q_{n, \alpha} \mid \phi\right\rangle$ in the Hilbert basis $\left\{\left|q_{n, \alpha}\right\rangle\right\}_{n \in \mathbb{Z}}$. This means that all physical kinematics and dynamics, i.e., that all relationships and maps between vectors in $D_{\text {physical }}$ can be described as relationships and maps between the coefficients of these vectors in the basis $\left\{\left|q_{n, \alpha}\right\rangle\right\}_{n \in \mathbb{Z}}$. The theory can therefore be viewed as a theory living on the discrete set of positions $\left\{q_{n, \alpha}\right\}_{n \in \mathbb{Z}}$ for some fixed $\alpha$. Nevertheless, this is not a discrete theory in the usual sense because the discretization is optional and one may freely change to describing the same physical dynamics and kinematics on any other grid of positions $\left\{q_{n, \alpha^{\prime}}\right\}$ for some other $\alpha^{\prime}$. This equivalence of a whole family of discrete representations of a theory is made possible by the fact that the finite lower bound $\Delta q_{\text {min }}$ makes these discretizations physically indistinguishable by any physical fields $|\phi\rangle \in D_{\text {physical }}$.

This mathematical structure provides a generalization of Shannon sampling theory, see [29], with $\Delta q_{\min }$ playing the role of a finite bandwidth. (Shannon sampling theory provides the link between discrete and continuous representations of information and it is used ubiquitously in signal processing and communication engineering.) The case $\alpha>0$ therefore describes a space which is simultaneously discrete and continuous in the same way that information can be continuous and discrete, see [30].

## 3. Back to generalized uncertainty relations

Our interest now will be to understand the interplay between lower bounds to position uncertainties and actual spatial discreteness in a way that is independent of representations and their functional analytic subtleties.

To analyze the relationship between a discrete length and coefficients in a generalized uncertainty principle, we here take a route on which we start with a conventional quantization of a fundamentally discrete quantum system. From this, we derive a generalized uncertainty principle of the form (8), with uniquely determined coefficients. Our methods will be
representation-independent, thus avoiding the need to address questions of superselection or domains. Although the example we study is simple, it should be able to serve as a model for analogous derivations to be performed if one wants to derive predictions for low-energy effects of fundamentally discrete systems, such as some versions of quantum gravity.

## III. QUANTUM MECHANICS ON A CIRCLE

In order to study the effects of the discreteness of the position, $q$, perturbatively, we will now use a simple system given by a quantized phase space of a cylinder where momentum $p$ has periodicity $p_{0}$, and derive uncertainty relations in an expansion by $p / p_{0}$. According to the discussion above, this is the regime of interest in quantum cosmology. The expansion can be done in a systematic and representation-independent way by computing higher moments of a state, and it provides specific coefficients which one can compare with the general form (8). Our techniques are motivated by a general scheme of effective equations in a canonical setting, which was developed in [32-34]. Such equations have been derived in loop quantum cosmology [35], for which the circle system provides a model capturing the characteristic representation. In fact, quantum mechanics on a circle can be seen as a sector in the Hilbert space of loop quantum cosmology, just as the set of all Bloch states is split into sectors of functions periodic up to phase. Being based on the same techniques, generalized uncertainty relations and effective equations may thus be combined for further phenomenological applications of quantum cosmology.

We present a brief overview of this simple well-known system in order to introduce our notation. Classical variables are a canonical pair $(q, p)$ with Poisson bracket $\{q, p\}=1$. In analogy with loop quantum cosmology we choose the momentum $p$ to be periodic, such that $p$ is the angle of a circle and thus takes values in $S^{1}$. Then, $q$ becomes discrete upon quantization. The phase space can be described by a complete set of phase space variables $\left(q, \sin \left(2 \pi p / p_{0}\right), \cos \left(2 \pi p / p_{0}\right)\right)$ where $p_{0}$ is the periodicity of $p$ which, $p$ being a dimensionless angle, can be fixed to $p_{0}=1$ but will be more useful for future expansions if kept unspecified. Instead of using the sine and cosine, it is more convenient to use the complex-valued function $h:=\exp \left(2 \pi i p / p_{0}\right)$ and its complex conjugate $h^{*}$, subject to the reality condition $h^{*} h=1$.

These basic functions satisfy the non-canonical algebra

$$
\begin{equation*}
\{q, h\}=\frac{2 \pi i}{p_{0}} h \quad, \quad\left\{q, h^{*}\right\}=-\frac{2 \pi i}{p_{0}} h^{*} \quad, \quad\left\{h, h^{*}\right\}=0 \tag{16}
\end{equation*}
$$

under taking Poisson brackets.
The quantum theory can be formulated on the Hilbert space $L^{2}\left(S^{1}, \mathrm{~d} p / p_{0}\right)$ which has an orthonormal basis $\{|n\rangle\}_{n \in \mathbb{N}}$, with momentum representation $\langle p \mid n\rangle=\exp \left(2 \pi i n p / p_{0}\right)$. The variable $q$ is directly quantized to become a multiplication operator acting by $\hat{q}|n\rangle=$ $2 \pi \hbar p_{0}^{-1} n|n\rangle$ which shows the discreteness of its spectrum. As before, wave functions need not be strictly periodic but could also be chosen periodic up to a phase: $\psi\left(p+p_{0}\right)=\exp (i \epsilon) \psi(p)$ with $\epsilon \in \mathbb{R}$. This is sufficient to ensure that the probability density is single-valued on the circle, and introduces a 1-parameter family of inequivalent representations for $\epsilon \in[0,2 \pi)$. They are inequivalent because the $\hat{q}$-spectrum possesses the eigenvalues $2 \pi \hbar(n+\epsilon) / p_{0}$ which depend on $\epsilon$. (We remark that we are now dealing with a closed circle instead of an interval with boundary conditions, so that non-strict periodicity may seem impossible to impose. Nevertheless, the corresponding Hilbert spaces can be formulated as function spaces on non-trivial line bundle over the circle, but we will not explicitly require these structures here.) There is no operator for $p$, however, because as a multiplication operator it would not map a basis state into another allowed state. Another way to see that such an operator cannot exist is to note that it would generate infinitesimal translations in $q$, which is not possible due to the discreteness of the $\hat{q}$-spectrum. There are, instead, well-defined operators for our basic functions $h$ and $h^{*}$, satisfying $\hat{h}|n\rangle=|n+1\rangle$ and $\widehat{h^{*}}|n\rangle=|n-1\rangle$. The reality condition for $p$ is satisfied since $\hat{h} \widehat{h}^{*}=\hat{1}$ and $\widehat{h^{*}}=\hat{h}^{\dagger}$.

## A. Moment algebra

Irrespective of the representation chosen, these basic operators satisfy the commutator algebra

$$
\begin{equation*}
[\hat{q}, \hat{h}]=-\frac{2 \pi \hbar}{p_{0}} \hat{h} \quad, \quad\left[\hat{q}, \hat{h}^{\dagger}\right]=\frac{2 \pi \hbar}{p_{0}} \hat{h}^{\dagger} \quad, \quad\left[\hat{h}, \hat{h}^{\dagger}\right]=0 \tag{17}
\end{equation*}
$$

which faithfully quantizes the classical basic algebra. The following calculations and our main results will make use only of this algebra and the reality condition, as well as the general Schwarz inequality; therefore they will be manifestly representation-independent.

Instead of working with wave functions as states, we will be using only the algebra (17) and functionals on it, suggestively characterized by expectation values $q=\langle\hat{q}\rangle, h=\langle\hat{h}\rangle$, $h^{*}=\left\langle\hat{h}^{\dagger}\right\rangle$ and moments

$$
\begin{equation*}
\Delta\left(q^{a} h^{b}\right):=\left\langle\left((\hat{q}-q)^{a}(\hat{h}-h)^{b}\right)_{\mathrm{Weyl}}\right\rangle \tag{18}
\end{equation*}
$$

of expectation values in Weyl ordering, where $a, b \in \mathbb{N}$ and $a+b \geq 2$. These variables form an (over-) complete set of functionals assigning complex numbers to the operators in our algebra. It follows from Hamburger's theorem that the probability density of a wave function can be reconstructed from the moments $\Delta\left(q^{n}\right)$, while the phase of the wave function can be found using moments involving $h$. For a pure state, the set of all moments is overcomplete. The additional freedom in the set of moments allows one to include mixed states as well.) The moments can be varied independently of expectation values to describe different states, provided they respect inequalities and reality conditions as discussed below. They are also useful for an analysis of coherent-state properties as e.g. in [36], which provides a link to the uncertainty relation. Our analysis here provides an independent and more direct relationship. From now on, we denote expectation values of basic operators by $q$ and $h$ without distinguishing them from the classical variables. This convention simplifies the notation and should not give rise to confusion.

Often, it is more convenient to work directly with equations for the moments rather than taking the detour of wave functions or density matrices, presenting a complete description from a more algebraic and representation-independent viewpoint. All crucial aspects of the system are then contained in the basic algebra, which in our case in particular means to use $\hat{h}$ as a basic operator on the circle, possibly combined with a Hamiltonian or a constraint. The main challenge then is to organize the infinitely many variables provided by the moments, and the equations of motion they must fulfill. An example where these equations can be organized in manageable ways is given by semiclassical regimes, in which moments of high order are small, but the treatment is not restricted to this case. Our approximation below will only assume the momentum (related to $h$ ) to be small compared to $p_{0}$, and any moments involving $p$ (relative to $p_{0}$ ) to fall off with increasing order as they do for semiclassical states but not only for such states; with these assumptions, fluctuations may still be large. Moreover, the size of the $q$-moments will remain unrestricted and need not be small compared to powers of $\hbar$. An advantage of the use of expectation values and
moments instead of wave functions is not only the representation independence but also its larger generality: it includes mixed states as well as pure ones.

We will be working mainly with moments of lower order where $a+b$ is small. For better clarity, we will then replace the superscript " $a, b$ " by a list of operators used in the moments. For instance, we have the $h$-variance $\Delta\left(h^{2}\right) \equiv(\Delta h)^{2}=: \Delta h^{2}$ and the covariance

$$
\Delta(q h)=\frac{1}{2}\langle(\hat{q}-q)(\hat{h}-h)+(\hat{h}-h)(\hat{q}-q)\rangle=\frac{1}{2}\langle\hat{q} \hat{h}+\hat{h} \hat{q}\rangle-q h .
$$

## B. Reality conditions

Expectation values and second-order moments are related to one another by the reality condition: taking an expectation value of the relation $\hat{h} \hat{h}^{\dagger}=\hat{1}$ implies

$$
\begin{equation*}
h h^{*}=1-\Delta\left(h h^{*}\right) \tag{19}
\end{equation*}
$$

This relation can be interpreted as reducing the number of independent expectation values of the basic variables to the canonical value two, such as $q$ and $\operatorname{Re}(h)$ (at fixed moments).

Similarly, at higher orders of the moments, we obtain additional reality conditions which reduce the number of moments to the canonical values as already used in [37]. For the second-order moments, we begin with the identities $\hat{h}^{2} \hat{h}^{\dagger}=\hat{h}$ and $\hat{q} \hat{h} \hat{h}^{\dagger}=\hat{q}$ that follow from $\hat{h} \hat{h}^{\dagger}=\hat{1}$, and take expectation values. With some symmetric reorderings according to the definition of the moments, we obtain

$$
\begin{align*}
h^{*} \Delta h^{2}+h \Delta\left(h h^{*}\right) & =-\Delta\left(h^{2} h^{*}\right)  \tag{20}\\
h^{*} \Delta(q h)+h \Delta\left(q h^{*}\right) & =-\Delta\left(q h h^{*}\right) . \tag{21}
\end{align*}
$$

The first equation is complex and implies two independent conditions for the moments, while the second equation is real. There are thus three conditions to restrict the secondorder moments (at fixed third-order ones) to the correct canonical number: out of six initial moments $\Delta q^{2}, \operatorname{Re} \Delta(q h), \operatorname{Im} \Delta(q h), \Delta\left(h h^{*}\right), \operatorname{Re} \Delta h^{2}$ and $\operatorname{Im} \Delta h^{2}$, three moments are left independent, amounting to two fluctuations and one correlation.

## C. Uncertainty relations

The main interest here lies in uncertainty relations which can be formulated in terms of the moments even if they are not used for a canonical pair $(q, p)$ but for a pair of our basic
operators. (See e.g. [36] for more details.) As usual, from the Schwarz inequality one derives

$$
\begin{equation*}
\Delta A^{2} \Delta B^{2}-\Delta(A B)^{2} \geq \frac{1}{4}\langle i[\hat{A}, \hat{B}]\rangle^{2} \tag{22}
\end{equation*}
$$

for any pair $(\hat{A}, \hat{B})$ of self-adjoint or symmetric operators. In our case, we can form three pairs of self-adjoint operators from the set $\left(\hat{q}, \hat{h}+\hat{h}^{\dagger}, i\left(\hat{h}-\hat{h}^{\dagger}\right)\right)$, giving uncertainty relations

$$
\begin{align*}
& \Delta q^{2} \Delta\left(h+h^{*}\right)^{2}-\Delta\left(q\left(h+h^{*}\right)\right)^{2}=2 \Delta q^{2}\left(\operatorname{Re} \Delta h^{2}+\Delta\left(h h^{*}\right)\right)-4(\operatorname{Re} \Delta(q h))^{2} \\
& \geq-\frac{\pi^{2} \hbar^{2}}{p_{0}^{2}}\left(h-h^{*}\right)^{2} \tag{23}
\end{align*}
$$

for $\hat{A}=\hat{q}$ and $\hat{B}=\hat{h}+\hat{h}^{\dagger}$,

$$
\begin{align*}
& \Delta q^{2} \Delta\left(i\left(h-h^{*}\right)\right)^{2}-\Delta\left(q i\left(h-h^{*}\right)\right)^{2}=2 \Delta q^{2}\left(-\operatorname{Re} \Delta h^{2}+\Delta\left(h h^{*}\right)\right)-4(\operatorname{Im} \Delta(q h))^{2} \\
& \geq \frac{\pi^{2} \hbar^{2}}{p_{0}^{2}}\left(h+h^{*}\right)^{2} \tag{24}
\end{align*}
$$

for $\hat{A}=\hat{q}$ and $\hat{B}=i\left(\hat{h}-\hat{h}^{\dagger}\right)$, and

$$
\begin{align*}
& \Delta\left(h+h^{*}\right)^{2} \Delta\left(i\left(h-h^{*}\right)\right)^{2}-\Delta\left(\left(h+h^{*}\right) i\left(h-h^{*}\right)\right)^{2} \\
& =4\left(\Delta\left(h h^{*}\right)^{2}-\left(\operatorname{Re} \Delta h^{2}\right)^{2}\right)-4\left(\operatorname{Im} \Delta h^{2}\right)^{2} \geq 0 \tag{25}
\end{align*}
$$

for $\hat{A}=\hat{h}+\hat{h}^{\dagger}$ and $\hat{B}=i\left(\hat{h}-\hat{h}^{\dagger}\right)$.
In semiclassical regimes, with moments of third or higher orders ignored, one can use the reality conditions to show that (24) implies (23) and (25). If moments of higher order are kept, (23) and (25) in combination with (24) and the reality conditions imply conditions for third-order moments, an example for higher-order uncertainty relations. For instance, (20), solved for $h^{*} \Delta h^{2}$ and then taken in its absolute value, implies

$$
|h|^{2}\left(\Delta\left(h h^{*}\right)^{2}-\left|\Delta h^{2}\right|^{2}\right)=-\left|\Delta\left(h^{2} h^{*}\right)\right|^{2}-2 \operatorname{Re}\left(h^{*} \Delta\left(h h^{*}\right) \Delta\left(h^{2} h^{*}\right)\right)
$$

and then

$$
\begin{equation*}
-2 \operatorname{Re}\left(h^{*} \Delta\left(h h^{*}\right) \Delta\left(h^{2} h^{*}\right)\right) \geq\left|\Delta\left(h^{2} h^{*}\right)\right|^{2} \tag{26}
\end{equation*}
$$

with (25).
Given that $\frac{i}{2}\left(\hat{h}-\hat{h}^{\dagger}\right)$ corresponds to the sine of $\hat{p}$, which should reduce to $\hat{p}$ when acting on states supported only on small $p$, we expect that it is (24) which reduces to the standard uncertainty relation when $p$ is small enough so that the periodicity can be ignored. To
confirm this expectation, we first consider only leading orders in the $p_{0}^{-1}$-expansion: we expand the operator

$$
\begin{equation*}
\hat{h}=1+\frac{2 \pi i}{p_{0}} \hat{p}-\frac{2 \pi^{2}}{p_{0}^{2}} \hat{p}^{2}+\cdots, \tag{27}
\end{equation*}
$$

which is valid on a set of states supported on values of $p$ small compared to $p_{0}$, and then compute the moments for the expansion. To leading order in $p_{0}^{-1}$, we need only the term $\hat{h}-h=2 \pi i p_{0}^{-1}(\hat{p}-p)+\cdots$, for which

$$
\begin{equation*}
\Delta\left(h h^{*}\right)=\left\langle(\hat{h}-h)\left(\hat{h}^{\dagger}-h^{*}\right)\right\rangle=\frac{4 \pi^{2}}{p_{0}^{2}} \Delta p^{2}+\cdots \tag{28}
\end{equation*}
$$

and

$$
\begin{equation*}
\Delta h^{2}=\left\langle(\hat{h}-h)^{2}\right\rangle=-\frac{4 \pi^{2}}{p_{0}^{2}} \Delta p^{2}+\cdots \tag{29}
\end{equation*}
$$

(As one can easily verify to this order, the reality condition $\Delta\left(h h^{*}\right)=1-|h|^{2}$ is identically satisfied in terms of the $p$-moments.)

For mixed moments we have to be more careful with the ordering:

$$
\begin{equation*}
\Delta(q h)=\frac{1}{2}\langle\hat{q} \hat{h}+\hat{h} \hat{q}\rangle-q h=\frac{i \pi}{p_{0}}\langle\hat{q} \hat{p}+\hat{p} \hat{q}\rangle-\frac{2 \pi i}{p_{0}} q p+\cdots=\frac{2 \pi i}{p_{0}} \Delta(q p)+\cdots . \tag{30}
\end{equation*}
$$

Inserting this in (24) provides the uncertainty product

$$
\begin{equation*}
2 \Delta q^{2}\left(\Delta\left(h h^{*}\right)-\operatorname{Re} \Delta h^{2}\right)-4(\operatorname{Im} \Delta(q h))^{2}=\frac{16 \pi^{2}}{p_{0}^{2}}\left(\Delta q^{2} \Delta p^{2}-\Delta(q p)^{2}\right)+\cdots \tag{31}
\end{equation*}
$$

which together with

$$
\frac{\pi^{2} \hbar^{2}}{p_{0}^{2}}\left(h+h^{*}\right)^{2}=\frac{4 \pi^{2} \hbar^{2}}{p_{0}^{2}}+\cdots
$$

results in the standard uncertainty relation

$$
\begin{equation*}
\Delta q^{2} \Delta p^{2}-\Delta(q p)^{2} \geq \frac{\hbar^{2}}{4} \tag{32}
\end{equation*}
$$

Equations (23) and (25) are satisfied identically to this order up to $p_{0}^{-2}$.

## D. Corrections to the uncertainty relation

Corrections do arise, however, if we expand to higher orders in $p_{0}^{-1}$, in which case we will obtain a generalized uncertainty relation as we demonstrate now. For instance, expanding to the next order on the right-hand side of the uncertainty relation (24) gives

$$
\begin{equation*}
\frac{1}{2}\left(h+h^{*}\right)=1-\frac{2 \pi^{2}}{p_{0}^{2}}\left(p^{2}+\Delta p^{2}\right)+\cdots . \tag{33}
\end{equation*}
$$

These corrections are identical to what would be obtained from a modified commutator of $\hat{q}$ and $\hat{p}$ as in (9), $[\hat{q}, \hat{\tilde{p}}]=i \hbar\left(1-2 \pi^{2} \hat{\tilde{p}}^{2} / p_{0}^{2}\right)$ with $\tilde{p}:=p_{0}\left(\hat{h}-\hat{h}^{\dagger}\right) / 2 \pi$, as it follows from a formal operator expansion

$$
\left[\hat{q}, \hat{h}-\hat{h}^{\dagger}\right]=\left[\hat{q}, \frac{4 \pi i \hat{p}}{p_{0}}-\frac{8 \pi^{3} i \hat{p}^{3}}{3 p_{0}^{3}}+\cdots\right]=-\frac{4 \pi \hbar}{p_{0}}\left(1-\frac{2 \pi^{2}}{p_{0}^{2}} \hat{p}^{2}+\cdots\right) .
$$

(This contribution to the corrected uncertainty relation for systems with compact configuration space is analogous to what is discussed in [38].)

However, the moments on the left-hand side of the uncertainty relation provide additional corrections to this order which must be included for a consistent expansion. Generalized uncertainty principles thus are not just consequences of modified commutators. We will need $\Delta(q h), \operatorname{Re} \Delta h^{2}$ and $\Delta\left(h h^{*}\right)$ up to the order $p_{0}^{-4}$ :

$$
\begin{align*}
\Delta\left(h h^{*}\right)= & \frac{4 \pi^{2}}{p_{0}^{2}} \Delta p^{2}-\frac{4 \pi^{4}}{3 p_{0}^{4}} \Delta\left(p^{4}\right)+\frac{4 \pi^{4}}{p_{0}^{4}}\left(\Delta p^{2}\right)^{2}+\frac{8 \pi^{4}}{p_{0}^{4}} p^{2} \Delta p^{2}  \tag{34}\\
\Delta h^{2}= & -\frac{4 \pi^{2}}{p_{0}^{2}} \Delta p^{2}-\frac{8 \pi^{3} i}{p_{0}^{3}} \Delta\left(p^{3}\right)-\frac{16 \pi^{3} i}{p_{0}^{3}} p \Delta p^{2} \\
& +\frac{28 \pi^{4}}{3 p_{0}^{4}} \Delta\left(p^{4}\right)+\frac{32 \pi^{4}}{p_{0}^{4}} p \Delta\left(p^{3}\right)-\frac{60 \pi^{4}}{p_{0}^{4}}\left(\Delta p^{2}\right)^{2}-\frac{24 \pi^{4}}{p_{0}^{4}} p^{2} \Delta p^{2}  \tag{35}\\
\Delta(q h)= & \frac{2 \pi i}{p_{0}} \Delta(q p)-\frac{2 \pi^{2}}{p_{0}^{2}} \Delta\left(q p^{2}\right)-\frac{4 \pi^{2}}{p_{0}^{2}} p \Delta(q p)-\frac{4 \pi^{3} i}{3 p_{0}^{3}} \Delta\left(q p^{3}\right)-\frac{4 \pi^{3} i}{p_{0}^{3}} p \Delta\left(q p^{2}\right)-\frac{4 \pi^{3} i}{p_{0}^{3}} p^{2} \Delta(q p) \\
& +\frac{2 \pi^{4}}{3 p_{0}^{4}}\left(\Delta\left(q p^{4}\right)+4 p \Delta\left(q p^{3}\right)+6 p^{2} \Delta\left(q p^{2}\right)+4 p^{3} \Delta(q p)\right) . \tag{36}
\end{align*}
$$

A demonstration of the lengthy calculations can be found in Appendix B. Moreover,

$$
\begin{equation*}
\Delta\left(h^{2} h^{*}\right)=\frac{8 \pi^{3} i}{p_{0}^{3}} \Delta\left(p^{3}\right)-\frac{8 \pi^{4}}{p_{0}^{4}}\left(\Delta\left(p^{4}\right)+2 p \Delta\left(p^{3}\right)-7\left(\Delta p^{2}\right)^{2}-6 p^{2} \Delta p^{2}\right) \tag{37}
\end{equation*}
$$

(One can verify that the reality condition (26) is identically satisfied in terms of the ( $q, p$ )moments.)

To this order, our three uncertainty relations read

$$
\begin{align*}
& \Delta q^{2} \Delta\left(p^{4}\right)+4 p \Delta q^{2} \Delta\left(p^{3}\right)-7 \Delta q^{2}\left(\Delta p^{2}\right)^{2}-2 p^{2} \Delta q^{2} \Delta p^{2} \\
& -4 p \Delta(q p) \Delta\left(q p^{2}\right)-\Delta\left(q p^{2}\right)^{2}-4 p^{2} \Delta(q p)^{2} \geq \hbar^{2} p^{2} \tag{38}
\end{align*}
$$

from (23),

$$
\begin{align*}
& \Delta q^{2} \Delta p^{2}-\Delta(q p)^{2}-\frac{4 \pi^{2}}{3 p_{0}^{2}}\left(\Delta q^{2} \Delta\left(p^{4}\right)+3 p \Delta q^{2} \Delta\left(p^{3}\right)-6 \Delta q^{2}\left(\Delta p^{2}\right)^{2}-3 p^{2} \Delta q^{2} \Delta p^{2}\right) \\
& -\frac{4 \pi^{2}}{3 p_{0}^{2}}\left(-\Delta(q p) \Delta\left(q p^{3}\right)-3 p \Delta(q p) \Delta\left(q p^{2}\right)-3 p^{2} \Delta(q p)^{2}\right) \geq \frac{\hbar^{2}}{4}\left(1-4 \pi^{2} \frac{p^{2}+\Delta p^{2}}{p_{0}^{2}}\right) \tag{39}
\end{align*}
$$

from (24), and

$$
\begin{equation*}
\Delta p^{2} \Delta\left(p^{4}\right)-\Delta\left(p^{3}\right)^{2}-7\left(\Delta p^{2}\right)^{3}-6 p^{2}\left(\Delta p^{2}\right)^{2} \geq 0 \tag{40}
\end{equation*}
$$

In order to eliminate some of the high-order moments in terms of second-order ones, we rewrite the three uncertainty relations as follows: (40) implies

$$
\begin{equation*}
\Delta_{1}:=\Delta\left(p^{4}\right)-7\left(\Delta p^{2}\right)^{2}-6 p^{2} \Delta p^{2} \geq \frac{\Delta\left(p^{3}\right)^{2}}{\Delta p^{2}} \geq 0 \tag{41}
\end{equation*}
$$

while (38) can be written as

$$
\begin{align*}
\Delta_{2}:= & \Delta q^{2}\left(\Delta\left(p^{4}\right)-7\left(\Delta p^{2}\right)^{2}-6 p^{2} \Delta p^{2}\right)+4 p \Delta q^{2} \Delta\left(p^{3}\right) \\
& +4 p^{2}\left(\Delta q^{2} \Delta p^{2}-\Delta(q p)^{2}-\hbar^{2} / 4\right)-4 p \Delta(q p) \Delta\left(q p^{2}\right) \geq \Delta\left(q p^{2}\right)^{2} \geq 0 \tag{42}
\end{align*}
$$

With the two non-negative quantities $\Delta_{1}$ and $\Delta_{2}$, the central uncertainty relation (39) reads

$$
\begin{align*}
& \Delta q^{2} \Delta p^{2}-\Delta(q p)^{2} \geq \frac{\hbar^{2}}{4}\left(1-4 \pi^{2} \frac{p^{2}+\Delta p^{2}}{p_{0}^{2}}\right) \\
& \quad+\frac{\pi^{2}}{p_{0}^{2}}\left(\Delta_{2}+\frac{1}{3} \Delta q^{2} \Delta_{1}+\hbar^{2} p^{2}+\frac{4}{3} \Delta q^{2}\left(\Delta p^{2}\right)^{2}-\frac{4}{3} \Delta(q p) \Delta\left(q p^{3}\right)\right) \\
& \geq  \tag{43}\\
& \frac{\hbar^{2}}{4}\left(1-\frac{4 \pi^{2}}{p_{0}^{2}}\left(\Delta p^{2}+\frac{4}{3} \frac{\Delta q^{2}\left(\Delta p^{2}\right)^{2}}{\hbar^{2}}-\frac{4}{3} \frac{\Delta(q p) \Delta\left(q p^{3}\right)}{\hbar^{2}}\right)\right)
\end{align*}
$$

using $\Delta_{1} \geq 0$ and $\Delta_{2} \geq 0$ (and $\Delta q^{2} \geq 0$ ) in the last step. If we assume that $\Delta(q p)=0$, only the remaining two fluctuations appear; all higher moments have been eliminated to order $p_{0}^{-4}$ in favor of additional fluctuation terms. Moreover, we can self-consistently insert the uncertainty relation on its right-hand side in (43) to bound $\Delta q^{2} \Delta p^{2}$ from below, resulting in the generalized uncertainty relation

$$
\begin{equation*}
\Delta q^{2} \Delta p^{2} \geq \frac{\hbar^{2}}{4}\left(1-\frac{16 \pi^{2}}{3 p_{0}^{2}} \Delta p^{2}\right) \tag{44}
\end{equation*}
$$

expanded to second order in $1 / p_{0}$. Taking a square root to this order, we have

$$
\begin{equation*}
\Delta q \Delta p \geq \frac{\hbar}{2}\left(1-\frac{8 \pi^{2}}{3} \frac{(\Delta p)^{2}}{p_{0}^{2}}\right) \tag{45}
\end{equation*}
$$

which is of the form (8) with a negative $\alpha=-8 \pi^{2} / 3 p_{0}^{2}$. We see that $\Delta q$ can vanish at a finite critical value of $\Delta p_{c}$, namely $\Delta p_{c}=\sqrt{-1 / \alpha}=\sqrt{3 / 2} p_{0} / 2 \pi$. While this value for $\Delta p_{c}$ shows the expected qualitative behavior, it can only be a rough estimate, given that the correction term $8 \pi^{3}\left(\Delta p_{c}\right)^{2} / 3 p_{0}$ is certainly not small when it cancels the standard term $\hbar / 2$ of the uncertainty relation. Nevertheless, the so-obtained value for the critical
$\Delta p_{c}$ is quite close to what we derived earlier for a position eigenstate. Our expansion by the moments assumes that all momentum variables, including the moments, are small compared to suitable powers of $p_{0}$, with $\Delta\left(p^{n}\right) / p_{0}^{n}$ falling off as $n$ gets larger. Even for $n=2$, the ratio is not small compared to one. For higher moments, as remarked at the end of Sec. IIA, position eigenstates (corresponding to $\Delta q=0$ ) do fulfill the fall-off assumption, but with a comparatively small rate of $2^{-n} /(n+1)$. (For comparison, semiclassical expansions usually make use of moments falling off as $\hbar^{n}$ relative to some classical scale with the dimension of an action, providing much smaller numbers.) Leaving position eigenstates aside, there is a large class of states that easily fulfill our assumptions provided they are sufficiently strongly peaked in $p$. For such states, our generalized uncertainty relation (45) reliably exhibits implications of discrete space on fluctuations.

## IV. CONCLUSIONS

We have derived the first order of corrections to the standard uncertainty relation as they result for a quantum system with a momentum space of the topology of $S^{1}$ and thus discrete position. Without needing to assume corrections to the basic operator algebra (17), we showed that an underlying discreteness of position spectra implies specific respresentationindependent correction terms in a generalized uncertainty principle. Formally, there is no self-adjoint operator associated with the coordinate of the compact direction of the phase space, which is rather quantized via periodic functions of an angular coordinate. (Grouptheoretical quantization [39], for instance, can be used to construct the quantum representation.) For angle separations small compared to the periodicity one can then expand quantum variables such as fluctuations, correlations and higher moments and, to leading order, reproduce the standard uncertainty relations. Higher orders of the expansion, which include terms sensitive to the periodicity, lead to a derived form of a generalized uncertainty principle.

Heuristically, a generalized uncertainty principle of a form that implies a positive lower bound for position uncertainty has been interpreted as a signal of spatial discreteness, as it may be realized in quantum gravity. This has been supported in [10] by an analysis of the representation theory of operator algebras which imply such a generalized uncertainty principle. Perhaps surprisingly, the specific form of the generalized uncertainty principle
derived in our calculations has the opposite sign of its coefficients compared to what leads to a finite minimal position uncertainty: Even though we know that the underlying Hilbert space implies discrete spectra and thus spatial discreteness in a rigorous sense, there is no finite lower bound to $\Delta q$.

Of course, as we discussed, one may expect the absolute minimum to be zero because normalizable eigenstates of sharp position exist. In this case, a more refined version of minimum uncertainty can be introduced which depends on the expectation value $\langle\hat{q}\rangle$ : the minimum uncertainty could vanish when $\langle\hat{q}\rangle$ equals an eigenvalue of $\hat{q}$, but would be non-zero otherwise. Such relations for the minimum $\Delta q_{\min }(\langle\hat{q}\rangle)$ can be derived at the Hilbert space level, but are not realized by the treatment used here. As we showed in Section II A, the presence of non-vanishing minima of fluctuations depends on the quantum representation. Generalized uncertainty principles, on the other hand, are representation independent as derived here; they follow from algebraic properties of quantum observables. While leading corrections to the standard uncertainty relation are $\langle\hat{q}\rangle$-independent and cannot directly give rise to minimal uncertainties of the functional form $\Delta q_{\min }(\langle\hat{q}\rangle)$, one may expect that higher orders could bring in such a dependence on $\langle\hat{q}\rangle$. Indeed, the dependence of $\Delta q_{\text {min }}$ on $\langle\hat{q}\rangle$ is most pronounced near $\hat{q}$-eigenstates, where the leading terms of the expansion in moments are not reliable. If higher orders are included, such a dependence may arise at least indirectly via moments involving $q$. These moments are independent of the expectation value, but specific classes of states, such as $\hat{q}$-eigenstates, could imply restrictions on the moments compatible with the form of $\Delta q_{\text {min }}$ seen before in (6). We leave this question open for future investigations.

Thus, there is no simple relationship between positive lower bounds for uncertainties according to generalized uncertainty principles on one hand, and true discreteness of operator spectra on the underlying Hilbert space on the other. One may view the existence of a positive lower bound for $\Delta q$ as an indication for a theory with a universal bandwidth, or a theory based on extended fundamental objects, which would be consistent with the fact that generalized uncertainty relations with a positive lower bound have been argued to arise, also from string theory. A key signature of a fundamental discreteness of space, by contrast, is the possibility of vanishing position fluctuations at finite momentum fluctuation. We reemphasize, however, that our treatment works well for values of variables small compared to their periodicity, for which curvature bounds in quantum gravity are an example. If one
instead probes an underlying periodic structure of position space, separations comparable to the periodicity scale would have to be considered where our present expansions do not apply.

As an alternative to string theory as a quantum theory of gravity, loop quantum gravity [40-42] provides a kinematical quantization where geometrical operators have discrete spectra [43, 44]. While this property has not been derived for physical observables, the discrete form of kinematical spectra affects the dynamics because of the form of basic operators which are combined to a Hamiltonian (constraint) operator. Dynamical implications can be studied in loop quantum cosmology [24-26], for instance in the context of space-time singularities [45]. The formulation of isotropic models in loop quantum cosmology makes use of complex exponentials of curvatures, rather than curvature components themselves [27]. The example analyzed here can thus be taken as a model for isotropic loop quantum cosmology, which indicates the form of generalized uncertainty principles as they may appear in cosmological applications. Our results here would apply only to small-curvature regimes where the discreteness of spatial geometry does not play a large role, corresponding to the fact that we had to expand our exponentials on a circle in the inverse periodicity in order to derive our generalized uncertainty principle.

Taking the circle example as a model for the kinematical structure of a sector in loop quantum cosmology suggests that the canonical variables $V$ and $P$, related to the volume and expansion rate as introduced in Appendix A, are subject to a generalized uncertainty principle

$$
\begin{equation*}
\Delta V \Delta P \geq \frac{\hbar}{2}\left(1-\frac{2}{3}(\Delta P)^{2}\right) \tag{46}
\end{equation*}
$$

This inequality is valid as long as $P$ and $\Delta P$ are small compared to the scale $P_{0}=2 \pi$ of almost periodicity. (As in the general derivation, we also assume a vanishing $(V, P)$ covariance; otherwise there will be additional corrections as shown by the previous formulas.) Loop quantum cosmology does not show uniquely what variables behave almost-periodically. Taking ambiguities into account, the periodicity scale in terms of the scale factor is set by two parameters $f_{0}$ and $x$ according to the power-law parameterization $P=-f_{0} a^{2 x} \dot{a}$. The dimension of $f_{0}$ depends on the value of $x$, given that $P$ must be dimensionless. For the value $x=-1 / 2$, for instance, $f_{0}$ has the dimension of length and due to its quantum-gravity origin one may expect it to be of the order of the Planck length $f_{0} \sim \ell_{\mathrm{P}}=\sqrt{G \hbar}$. (For consistency with other corrections from loop quantum cosmology, it must be sufficiently larger than the

Planck length [46].) In this case, a Planckian bound $\dot{a} / a<\ell_{\mathrm{P}}^{-1}$ for the Hubble parameter is required for the applicability of our derivations here and leading corrections are of the order $\left(\ell_{\mathrm{P}} \Delta(\dot{a} / a)\right)^{2}$.

In fact, as observed in [47], the use of modified commutation relations between the canonical variables which correspond to a generalized uncertainty principle of the form derived here can mimic some of the effects of loop quantum cosmology. The main example is a bounce in isotropic models sourced by a free scalar [35, 48]. However, such an example for high-curvature effects appears when $P \sim P_{0}$ and thus falls outside the regime where derivations of the present paper are valid. We nevertheless note that our derivations are not restricted to purely semiclassical regimes; all we need is a hierarchy of moments organized by powers of $P_{0}^{-1}$, not of $\hbar$.

In addition to the gravitational degrees of freedom, loop quantization also applies to matter fields. A scalar field, for instance, can be represented on the loop Hilbert space in an almost-periodic fashion similar to the gravitational connection or the canonical variable $P$ in isotropic cosmology [49, 50]. In a setting of quantum field theory, generalized uncertainty relations should then appear, with possible phenomenological consequences during inflation.

Let us recall that our considerations here have been kinematical, using a moment expansion in uncertainties. The same tool is the key to analyzing quantum back-reaction effects in the dynamics, where equations of motion (or constraints) are expanded by moments [32]. This can be done either in canonical variables or in variables analogous to $h$ used on the circle [35]. We leave it open to further studies to see what a combination of both types of moment expansions would provide.

Finally, let us consider how the present considerationsl could be extended to account for particle interactions. There are in principle two approaches, bottom up and top down. In the top down approach, a multi particle version of the present considerations is provided by any top level quantum gravity theory such as loop quantum gravity, which then yields a single particle generalized uncertainty principle in a suitable limit. In the bottom up approach, one can try to extend generalized uncertainty principles to a multi particle theory. For example, in the case of a constant finite minimum uncertainty in position, e.g. at the Planck scale, the space of fields is known to be bandlimited with the smallest wavelength determined by the minimum length uncertainty. A quantum field theory is then obtained by taking an ordinary quantum field theoretical path integral and restricting the integration range to just these
bandlimited functions, thereby in effect eliminating the most extreme quantum fluctuations. This approach has been pursued, for example, in [29]. The bottom-up approach then also encounters the question of the addition of momenta, see for example [13]. For example, when multiple bandlimited functions are multiplied naively to describe the scattering of multiple particles, the product of these functions need not obey the same bandlimit. Indeed, when particles scatter whose combined energy reaches or exceeds the Planck energy then their interaction with the background spacetime must become strong. It is plausible that this interaction could lead to a transfer of excess momentum to curvature degrees of freedom, thereby resolving the issue of the conservation of the momenta and of the bandlimitation. These questions are beyond the scope of the present paper.

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## Appendix A: Loop quantum cosmology

We present a brief review of loop quantum cosmology with a focus on aspects relevant for questions of the discreteness or periodicity of some directions in phase space. In this context, we must take a general viewpoint in order to see all possible forms of discreteness that can arise, especially at a dynamical level. Our summary here therefore differs from some contributions and reviews in the recent literature, where models are specialized further by ad-hoc choices so as to produce detailed studies of some specific cases.

In loop quantum gravity [40-42], one uses as one of the basic canonical fields a densitized triad $E_{i}^{a}$ of three orthonormal vector fields labelled by $i=1,2,3$, related to the spatial metric $q_{a b}$ by $E_{i}^{a} E_{i}^{b}=\sqrt{\operatorname{det} q} q^{a b}$. As a smeared version, the field is quantized via flux operators $\hat{F}(S)=\int_{S} \hat{E}_{i}^{a} n_{a} \mathrm{~d}^{2} y$ integrated over 2-dimensional surfaces in space rather than by its pointwise values. In an isotropic setting, $E_{i}^{a}=p \delta_{i}^{a}$ is completely determined by the scale factor $a$ up to orientation, with $|p|=a^{2}$ and the sign of $p$ giving the orientation of space. Fluxes, then, reduce to area-like quantities such as $A=\ell_{0}^{2}|p|$ where $\ell_{0}$ provides a
linear measure (in terms of coordinates) for the surfaces used.
In quantum states, areas $A$ obtained from flux operators play the role of quantum numbers that determine the elementary discreteness of space. Indeed, the quantum representation implies a discrete spectrum for flux operators, whose smallest possible non-zero values are of the order $A \sim \ell_{\mathrm{p}}^{2}$. One is thus led to a discrete (minisuper)space as used in this article. For isotropic geometries, the canonically conjugate almost-periodic momentum of $A$ is $\ell_{0} \dot{a}$ (represented via holonomy operators). But while the spectrum of flux operators for fixed surfaces is fully determined and of a simple equidistant form, the question of what the dynamical stepsize of physical scales is, for instance in an expanding universe, remains open. The dynamics of a classical expanding universe is described by the scale factor or the triad variable $p$, while elementary fluxes in quantum theory determine the possible sizes of $\ell_{0}^{2}|p|$ with $\ell_{0}$ depending on the coordinate size of surfaces (or plaquettes in a lattice-like state of discrete space) giving rise to the smallest flux eigenvalues. If the lattice is changing, a process called lattice refinement which is generically realized in loop quantum gravity [51, 52], $\ell_{0}$ must be assumed to depend on time or the scale factor as well. The known equidistant spectrum for fluxes $A$ then determines the stepsize of geometrical measures related to the scale factor only if $\ell_{0}$ for lattice plaquettes is known as a function of $a$ or $p$.

Evaluating the full dynamics of loop quantum gravity, for instance as in [53], remains extremely challenging; it is thus impossible to derive some function $\ell_{0}(p)$ from first principles. However, on general grounds there are certain restrictions on its behavior. If $\ell_{0}$ did not depend on $p$, for instance, the discreteness scale of a lattice state would be constant in terms of coordinates, but would be magnified as the scale $a \ell_{0}$ measured in an expanding universe. For sufficiently long expansion, one would be in conflict with continuum physics. A decreasing scale $\ell_{0}(p)$ is thus required, one useful example being the power-law form $\ell_{0}(p)=f_{0}|p|^{x}$ with two constants $f_{0}$ for the discreteness scale and $x<0$ for the refinement behavior. It is then the product $\ell_{0}(p) \dot{a}=f_{0} a^{2 x} \dot{a}$, not $\dot{a}$, which is almost periodic, and the conjugate variable $\int \ell_{0}(p)^{-1} \mathrm{~d} p=f_{0}^{-1}|p|^{1-x} /(1-x)$, not $p$, which is equidistant.

In terms of the cosmological scale factor $a$, we thus define canonical variables

$$
\begin{equation*}
V=\frac{3 \sigma \mathcal{V} a^{2-2 x}}{8 \pi G(1-x) f_{0}} \quad \text { and } \quad P=-f_{0} a^{2 x} \dot{a} \quad \text { with } \quad\{V, P\}=1 \tag{A1}
\end{equation*}
$$

where $G$ is the gravitational constant. These conventional variables absorb the precise periodicity scale of $a^{2 x} \dot{a}$ in $f_{0}$ such that $P_{0}=2 \pi$ and $\mu_{n}^{(\epsilon)}=n+\epsilon / 2 \pi$. In $V$, moreover,
the spatial volume $\mathcal{V}$ of an integration region used to average to isotropy, measured in coordinates, appears, as well as $\sigma= \pm 1$ which determines the orientation of space. With the factor of $\sigma$, allowed values of $V$ cover the whole real line because loop variables are derived from triads, which by changing orientation can take both signs; see [25] for derivations and details.

The dynamics of a loop quantum cosmological model takes different forms depending on which variable precisely is almost periodic. Unlike the condensed-matter example in Section II, it is not clear a priori whether it is, say, $a$ itself which acquires an equidistant spectrum in any of the periodic dynamical sectors, or a different power of $a$ (or yet another functional behavior). We therefore keep this freedom in our definition of basic variables where the power $x$ remains unspecified. (Arguments loosely based on the full theory of loop quantum gravity indicate that $-1 / 2<x<0$ generically [51, 52], with values near $-1 / 2$ preferred phenomenologically [54-56] at least in near-isotropic cosmology.) Moreover, even if the precise discrete variable would be specified, the discreteness scale remains free. This is parameterized by the second constant $f_{0}$ whose dimension depends on $x$.[66]

A further difference to the Bloch example is that this so-called kinematical Hilbert space of states (4), as it follows[67] from the full theory of loop quantum gravity, carries a different representation than is typically used in quantum mechanics [28]: All states $\psi_{n}^{(\epsilon)}$ are normalizable despite their plane-wave form, and they form an orthonormal basis. (Although non-standard, this representation may be advantageously used also in quantum mechanics [61] and quantum field theory [62].) Since there are uncountably many such states, the Hilbert space is non-separable. A specific way to write the inner product is the integral form

$$
\begin{equation*}
\langle f, g\rangle=\lim _{T \rightarrow \infty} \frac{1}{2 T} \int_{-T}^{T} \overline{f(P)} g(P) \mathrm{d} P \tag{A2}
\end{equation*}
$$

Since $V$ is conjugate to $P$, it can be represented as the usual derivative operator $\hat{V}=$ $i \hbar \partial / \partial P$. The states (4) then turn out to be true normalizable eigenstates of $\hat{V}$, which thus has a discrete spectrum. For the scale factor $a$, the eigenvalues in terms of the quantum number $\mu_{n}^{(\epsilon)}$ read

$$
\begin{equation*}
a_{n}^{(\epsilon)}=\left(\frac{8 \pi G \hbar f_{0}(1-x)\left|\mu_{n}^{(\epsilon)}\right|}{3 \mathcal{V}}\right)^{1 /(2-2 x)}=\left(\frac{8 \pi G \hbar f_{0}(1-x)|n+\epsilon / 2 \pi|}{3 \mathcal{V}}\right)^{1 /(2-2 x)} \tag{A3}
\end{equation*}
$$

As in the case of Bloch states, it is the dynamics which must determine the specific realiza-
tion and effects of the underlying discreteness as well as potentially observable implications. Classically, cosmological dynamics is governed by the Friedmann equation

$$
\begin{equation*}
0=C=a \dot{a}^{2}-\frac{8 \pi G}{3} E(a) \tag{A4}
\end{equation*}
$$

where $a$ is the scale factor and $E$ the matter energy in the universe. Since $\dot{a}$, according to (A1) is related to the variable $P$ which, after a loop quantization, becomes almost periodic, it is not possible to represent the Friedmann equation directly on the Hilbert space of loop quantum cosmology. Instead, one has to look for an operator which is well-defined and which produces $\dot{a}^{2}$ in the classical limit of small curvature where $\dot{a} \ll 1$ (or more precisely $f_{0} a^{2 x} \dot{a} \ll 1$ ). With $P$ parameterized to reflect the scale of almost periodicity, a simple and often-used operator that satisfies the requirements is obtained after replacing $a \dot{a}^{2}$ in (A4) with $f_{0}^{-2} a^{1-4 x} \sin ^{2} P$ where $a^{1-4 x}$ is proportional to $V^{2-3 /(2-2 x)}$ in terms of canonical variables. This specific process of adapting the classical equation in large-curvature regimes is called "holonomy modification." It plays the role of a regularization to ensure that the classical expression can be promoted to an operator in the quantum representation used.

A detailed derivation of the precise functional form of the Hamiltonian, or the specific form of functions such as $\sin ^{2} P$ in holonomy modifications, must await further developments in evaluating the theory. This would be like asking to derive the potential $V(x)$ relevant for the motion of electrons in a crystal from first principles of the underlying many-body system composed of all nuclei and electrons. Such a derivation is certainly complicated, but still the Hamiltonian resulting from the simple basic assumptions made above has several characteristic properties for which the detailed form is not crucial. They influence the dynamics, which in qualitative terms will depend on the size of parameters such as $f_{0}$ and $x$. In contrast to a condensed-matter Hamiltonian, in this context one is not interested in all energy eigenvalues but only in the zero eigenspace, so-called physical states annihilated by the combined Hamiltonian of gravity and matter which forms a constraint rather than an expression of energy. There is thus no band structure, but implications of the discreteness do show up in other dynamical properties of the solutions.

From the action of a holonomy modification like $\sin ^{2} P$ as a multiplication operator

$$
\begin{equation*}
\widehat{\sin ^{2} P} \psi_{n}^{(\epsilon)}(P)=-\frac{1}{4}\left(\psi_{n+2}^{(\epsilon)}(P)-2 \psi_{n}^{(\epsilon)}(P)+\psi_{n-2}^{(\epsilon)}(P)\right) \tag{A5}
\end{equation*}
$$

on $\hat{V}$-eigenstates $\psi_{n}^{(\epsilon)}$ of the form (4), with a matter Hamiltonian operator $\hat{E} \psi_{n}^{(\epsilon)}(P)=$
$E_{n}^{(\epsilon)} \psi_{n}^{(\epsilon)}(P)$, the constraint $C=0$ in (A4) is quantized to a difference equation $[27,63]$

$$
\begin{equation*}
C_{+}^{(\epsilon)}(n) s_{n+2}^{(\epsilon)}+C_{0}^{(\epsilon)}(n) s_{n}^{(\epsilon)}+C_{-}^{(\epsilon)}(n) s_{n-2}^{(\epsilon)}=\frac{8 \pi G}{3} E_{n}^{(\epsilon)} s_{n}^{(\epsilon)} \tag{A6}
\end{equation*}
$$

for the coefficients of physical states $\psi(P)=\sum_{n, \epsilon} s_{n}^{(\epsilon)} \psi_{n}^{(\epsilon)}(P)$ expanded in (4). The coefficients $C_{0}^{(\epsilon)}(n)$ and $C_{ \pm}^{(\epsilon)}(n)$ of the difference equation follow from quantizing the $a$-dependent terms in (A4); see e.g. [25, 27, 64] for concrete examples. Eq. (A6) may appear like an eigenvalue equation for $E_{n}^{(\epsilon)}$, but solutions to this constraint are not required to be normalizable. In fact, if the system describes an ever-expanding cosmology, wave functions are expected to be supported at all $n$ without a strong fall-off at $n \rightarrow \pm \infty$. Thus, general solutions are not normalizable. However, they describe the change of the wave function of an evolving universe for any given $\hat{E}$ in accordance with the matter model.

## Appendix B: Example for the expansion of moments

Here we show some of the calculations necessary to expand moments up to third order in $p_{0}^{-1}$. In the main text, we had to use results up to fourth order, which are more lengthy but follow from analogous calculations.

First, we have

$$
\begin{equation*}
\Delta h^{2}=\left\langle\hat{h}^{2}\right\rangle-h^{2}=-\frac{4 \pi^{2}}{p_{0}^{2}} \Delta p^{2}-\frac{8 \pi^{3} i}{p_{0}^{3}} \Delta\left(p^{3}\right)-\frac{16 \pi^{3} i}{p_{0}^{3}} p \Delta p^{2}+\cdots \tag{B1}
\end{equation*}
$$

where we used the third-order moment

$$
\begin{equation*}
\Delta\left(p^{3}\right)=\left\langle(\hat{p}-p)^{3}\right\rangle=\left\langle\hat{p}^{3}\right\rangle-3 p\left\langle\hat{p}^{2}\right\rangle+2 p^{3} . \tag{B2}
\end{equation*}
$$

For mixed moments we have to be more careful with the ordering:

$$
\begin{align*}
\Delta(q h) & =\frac{1}{2}\langle\hat{q} \hat{h}+\hat{h} \hat{q}\rangle-q h  \tag{B3}\\
& =\frac{i \pi}{p_{0}}\langle\hat{q} \hat{p}+\hat{p} \hat{q}\rangle-\frac{2 \pi i}{p_{0}} q p-\frac{\pi^{2}}{p_{0}^{2}}\left\langle\hat{q} \hat{p}^{2}+\hat{p}^{2} \hat{q}\right\rangle+\frac{2 \pi^{2}}{p_{0}^{2}} q\left\langle\hat{p}^{2}\right\rangle-\frac{2 \pi^{3} i}{3 p_{0}^{3}}\left\langle\hat{q} \hat{p}^{3}+\hat{p}^{3} \hat{q}\right\rangle+\frac{4 \pi^{3} i}{3 p_{0}^{3}} q\left\langle\hat{p}^{3}\right\rangle+\cdots \\
& =\frac{2 \pi i}{p_{0}} \Delta(q p)-\frac{2 \pi^{2}}{p_{0}^{2}} \Delta\left(q p^{2}\right)+\frac{4 \pi^{2}}{p_{0}^{2}} p \Delta(q p)-\frac{4 \pi^{3} i}{3 p_{0}^{3}} \Delta\left(q p^{3}\right)-\frac{4 \pi^{3} i}{p_{0}^{3}} p \Delta\left(q p^{2}\right)-\frac{4 \pi^{3} i}{p_{0}^{3}} p^{2} \Delta(q p)+\cdots
\end{align*}
$$

where in the last step the moments
$\Delta\left(q p^{2}\right)=\frac{1}{3}\left\langle(\hat{q}-q)(\hat{p}-p)^{2}+(\hat{p}-p)(\hat{q}-q)(\hat{p}-p)+(\hat{p}-p)^{2}(\hat{q}-q)\right\rangle$

$$
\begin{align*}
& =\frac{1}{2}\left\langle\hat{q} \hat{p}^{2}+\hat{p}^{2} \hat{q}\right\rangle-q \Delta p^{2}-2 p \Delta(q p)-q p^{2}  \tag{B4}\\
\Delta\left(q p^{3}\right) & =\frac{1}{4}\left\langle(\hat{q}-q)(\hat{p}-p)^{3}+(\hat{p}-p)(\hat{q}-q)(\hat{p}-p)^{2}+(\hat{p}-p)^{2}(\hat{q}-q)(\hat{p}-p)+(\hat{p}-p)^{3}(\hat{q}-q)\right\rangle \\
& =\frac{1}{2}\left\langle\hat{q} \hat{p}^{3}+\hat{p}^{3} \hat{q}\right\rangle-q \Delta\left(p^{3}\right)-3 p \Delta\left(q p^{2}\right)-3 p^{2} \Delta(q p)-q p^{3} \tag{B5}
\end{align*}
$$

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[65] Another difference (but one not relevant here) is that $\bigoplus_{\epsilon} \mathcal{H}_{\epsilon}$ is taken as the full Hilbert space of the model, with all states (4) normalizable. One can view these wave functions as being supported on the Bohr compactification of the real line [28], with an invariant measure that differs from the one usually used in quantum mechanics. At this level, one is dealing with a non-separable Hilbert space, but superselection is often introduced at the dynamical level. Then, one can again assume fixed $\epsilon$ without loss of generality.
[66] In this context, one should be careful due to the scaling behavior of $a$ : as the scale factor of a universe, its value changes whenever spatial coordinates are rescaled by a constant. Thus, $f_{0}$ is not coordinate independent (unless $x=-1 / 2$ ) because it must absorb the coordinate dependence of the scale factor. For a similar reason, $f_{0}$ depends on the spatial averaging volume $\mathcal{V}$ which is not only coordinate dependent but also changes whenever a different integration region is chosen. Both dependences of $f_{0}$ are only artefacts of the isotropic formulation in terms of the scale factor, and do not imply that the physical model would depend on coordinates or the choice of an integration region. (The scaling issue is not altogether avoided in spatially closed models with their compact total space because one may still use regions smaller than the total space for averaging to isotropy.)
[67] There are different ways to derive the basic representation on the kinematical Hilbert space
from full loop quantum gravity [51, 57-60]. The derivation of dynamics via a reduced Hamiltonian constraint operator from a full one is, however, more complicated. If this could be done in sufficient detail, the parameters $f_{0}$ and $x$ could in principle be determined.

