We present a study of the evolution of entanglement entropy of matter and geometry in quantum cosmology. For a variety of initial quantum states of the Universe, and with evolution defined with respect to a relational time, we show numerically that (i) entanglement entropy increases rapidly at very early times, and subsequently saturates to a constant non-zero value, and (ii) that the saturation value of this entropy is a linear function of the energy associated to the quantum state: $S_{\text{ent}}^\gamma = \gamma (\mathcal{H}|\psi\rangle$. These results suggest a remnant of quantum entanglement in the macroscopic Universe from the era of the Big Bang, independent of the initial state, and a “First Law” associated with matter-gravity entanglement entropy in quantum gravity.

**Introduction** The system of two spin one-half particles is the simplest example of a bipartite system in quantum mechanics. The notions of product states, entangled states (Bell pairs), and the Von-Neumann entanglement entropy are readily illustrated in this 4-dimensional Hilbert space $\mathcal{H} = \mathcal{H}_1^{(1)} \times \mathcal{H}_2^{(2)}$.

Time evolution of entanglement entropy may be computed for a state for a given Hamiltonian $H$. This may be illustrated for example with the Hamiltonian

$$
H = \sigma_z^{(1)} \otimes I^{(2)} + I^{(1)} \otimes \sigma_z^{(2)} + g (\sigma_z^{(1)} \otimes \sigma_z^{(2)} + \sigma_+^{(1)} \otimes \sigma_+^{(2)}),
$$

(1)

where $I^{(1)}, I^{(2)}$ are the identity matrices in each component Hilbert space, $\sigma_z$ is the diagonal Pauli matrix, $\sigma_z = \sigma_x \pm i \sigma_y$, and $g$ is a coupling constant. It is easily verified that an exact solution of the time-dependent Schrodinger equation for this Hamiltonian is

$$
|\psi\rangle = \cos(gt)|01\rangle - i \sin(gt)|10\rangle
$$

(2)

(in the usual notation for a two state system where $|01\rangle \equiv |0\rangle \otimes |1\rangle$). With $\rho = |\psi\rangle \langle \psi|$ and $\rho_1 = \text{Tr}_2(\rho)$, the entanglement entropy associated to this state is

$$
S_{\text{ent}}(g, t) \equiv -\text{Tr}(\rho_1 \log \rho_1)
= -\cos^2(gt) \ln[\cos^2(gt)] - \sin^2(gt) \ln[\sin^2(gt)].
$$

(3)

This simple result has two noteworthy features: the entropy oscillates between zero and its maximum possible value ($\ln 2$), and in the decoupling limit, $\lim_{g \to 0} S_{\text{ent}}(g, t) = 0$.

This elementary example provides a prototype for the quantum gravity (QG) calculation we present here. Before we proceed to develop this, let us first note that general relativity (GR) coupled to matter naturally provides at least a “bipartite” system without any externally imposed separation of regions of space as in single field cases where entanglement between regions of space are studied [1–4]: the physical Hilbert space is naturally a tensor product of the geometry ($G$) and matter ($M$) components $\mathcal{H} = \mathcal{H}_G \otimes \mathcal{H}_M$, since these are independent degrees of freedom already in the classical theory. If there is more than one species of matter, $\mathcal{H}_M$ would be a tensor product of the Hilbert spaces of the individual matter species. This observation holds regardless of the specific approach to QG. (Related comments concerning this decomposition of QG. (Related comments concerning this decomposition of the Hilbert space appear in [5]). Secondly, there is no obvious physical “Hamiltonian” for GR; instead canonical GR provides a hamiltonian constraint that generates “time evolution” as the gauge transformation associated to time reparametrization invariance.

This feature, common to every theory with time reparametrization invariance, has given rise two distinct approaches to non-perturbative QG, known as Dirac and reduced phase space quantization. In the former approach, physical states are determined by solving the timeless (Wheeler-deWitt) constraint equation $\hat{\mathcal{H}}|\Psi\rangle = 0$. In the latter approach, all gauges are fixed classically before quantization (for reviews of QG see eg. [7, 8]. The second approach gives a non-vanishing physical Hamiltonian which may then be quantized as in a theory without constraints. (A comparison of the two approaches appears in [9, 10].)

Our purpose is to investigate two questions. How does matter-geometry entanglement entropy evolve in quantum gravity? And does entanglement remain in a macroscopic Universe? These questions provide a first probe of questions such as the emergence of a classical Universe from quantum gravity and of quantum fields in curved spacetime. To study these questions we consider the simpler setting of homogeneous and isotropic cosmology. Although there have been numerous studies in quantum cosmology over the years [11–17], to our knowledge there is no other work on the two specific questions we address in this work in the context of QG. There is however a conjecture that the entropy of a (closed) quantum gravity system is the matter-geometry entanglement entropy [5]; this work does not give a computation of entanglement entropy evolution, which requires a notion of time. Our work here does not address this conjecture. Another
recent work gives a study entanglement entropy evolution in non-gravitational systems [18].

We use a partially reduced phase space quantization with GR coupled to dust and a scalar field, where the dust field is used as a clock, and obtain the corresponding physical Hamiltonian [19–21]. With the dust thereby removed as a dynamical variable, this Hamiltonian is in general a functional of the spatial metric \(q_{ab}\), scalar field \(\phi\), and their canonically conjugate momenta. When applied to cosmology, this procedure gives a time dependent Schrodinger equation for evolving arbitrary states \(\psi(q, \phi, t = 0)\) specified as initial data.

We compute numerically the evolution for a variety of initial states (including “multiverse” linear combinations), and thereby derive the time evolution of matter-geometry entanglement entropy in the very early quantum Universe. Our main result are (i) that entanglement entropy increases rapidly and saturates to a non-zero constant that is dependent on the initial data, and (ii) the saturation value of the entanglement entropy is a linear function of the expectation value of the Hamiltonian. Taken together these results are remarkable in that they constitute a “First Law” for matter-gravity entanglement entropy in quantum gravity.

**Model and quantization** Let us first recall the classical theory. The action is [20]

\[
S = -\frac{1}{8\pi G} \int d^4x \sqrt{-g} R + \int d^4x \sqrt{-g} g^{ab} \partial_a \phi \partial_b \phi
+ \int d^4x \sqrt{-g} \left( m \left( g^{\mu\nu} \partial_{\mu} T \partial_{\nu} T + 1 \right) \right),
\]

where \(T\) and \(\phi\) are the dust and scalar fields. The last term is the pressureless dust action; its variation with respect to \(m\) gives the condition that \(T\) has time-like gradient. (We use units where \(G = c = \hbar = 1\). The canonical theory obtained from this action is

\[
S = \int dt d^3x \left( \hat{\pi}^{ab} \dot{q}_{ab} + p_\phi \dot{\phi} + \rho T - NH - Na \right),
\]

where the pair \((q_{ab}, \hat{\pi}^{ab})\) is the Arnowitt-Deser-Misner (ADM) phase space variables of GR, and \((T, p_T)\) and \((\phi, p_\phi)\) are respectively the phase space variables of the scalar and dust fields. The lapse and shift functions, \(N\) and \(N^a\) are the coefficients of the Hamiltonian and diffeomorphism constraints

\[
\mathcal{H} = \mathcal{H}^G + \mathcal{H}^D + \mathcal{H}^\phi,
\]

\[
\mathcal{C}_a = -2D_b \hat{\pi}^{ba} + p_T \partial_a T + p_\phi \partial_a \phi;
\]

\(\mathcal{H}^G\) and \(\mathcal{H}^\phi\) are the familiar gravitational and scalar field parts of the ADM Hamiltonian constraint, and

\[
\mathcal{H}^D = \frac{1}{2} \left( \frac{p_T^2}{m \sqrt{q}} + m \sqrt{q} (q^{ab} \partial_a T \partial_b T + 1) \right).
\]

The momentum conjugate to the field \(m\) is zero since it appears as a Lagrange multiplier in the covariant action. At this point one could enlarge the phase space to treat \(m\) and its conjugate momentum as independent degrees of freedom, subsequently eliminating them by gauge fixing. However, it is more straightforward to vary the term \(\mathcal{H}^D\) in the canonical action with respect to \(m\), and use the resulting equation of motion:

\[
m = \pm \frac{p_T}{\sqrt{q} (q^{ab} \partial_a T \partial_b T + 1)}.
\]

This can then be substituted back into \(\mathcal{H}^D\) to give

\[
\mathcal{H}^D = sgn(m) \rho T \sqrt{q^{ab} \partial_a T \partial_b T + 1}.
\]

The resulting action is a functional of only the canonical pairs \((q_{ab}, \hat{\pi}^{ab}), (T, p_T)\) and \((\phi, p_\phi)\). It is readily verified that the constraints remain first class with this elimination of \(m\).

We now partially reduce the theory by fixing only a time gauge, and solving the Hamiltonian constraint to obtain a physical Hamiltonian. The spatial coordinates remain unfixed. We use the dust time gauge [20] which equates the physical time with the dust field \(T\) field,

\[
\lambda \equiv T - \epsilon t \approx 0, \quad \epsilon = \pm 1.
\]

The condition (11) has a nonzero Poisson bracket with the Hamiltonian constraint, so this pair of constraints together is second class. A gauge condition is considered suitable if the matrix of Poisson brackets of second class constraints is invertible. The first of these gives, using (10), the Dirac matrix of second class constraints

\[
C = \begin{bmatrix} 0 & \{\lambda, \mathcal{H}\} \\ \{\mathcal{H}, \lambda\} & 0 \end{bmatrix} = \begin{bmatrix} 0 & 1 \\ -1 & 0 \end{bmatrix}.
\]

This matrix is invertible everywhere on the manifold. Thus, the dust time gauge does not breakdown at any point and is therefore a robust choice. The second condition, requiring that the gauge condition be preserved in time, gives an equation for the lapse function:

\[
\epsilon = \dot{T} = \left. \left( \int d^3x \left( N \mathcal{H} + N^a \mathcal{C}_a \right) \right) \right|_{T = t} = sgn(m) N.
\]

The corresponding physical Hamiltonian density is

\[
\mathcal{H}_P = -\epsilon p_T = sgn(m) \epsilon \left( \mathcal{H}^G + \mathcal{H}^\phi \right) = N \left( \mathcal{H}^G + \mathcal{H}^\phi \right),
\]

where the second equality follows from solving the Hamiltonian constraint and the third using (13). We also note that the definition of \(p_T\) from the dust action, in this gauge, gives

\[
p_T = \frac{m}{N} \sqrt{q} \dot{T} = sgn(m) \epsilon \left| \frac{m}{N} \sqrt{q} = |m| \sqrt{q} > 0 \right.
\]

In the following we work with \(N = 1\). Substituting into Eq. (5) gives the gauge fixed action

\[
S^{GF} = \int dt d^3x \left[ \hat{\pi}^{ab} \dot{q}_{ab} + p_\phi \dot{\phi} + (\mathcal{H}^G + \mathcal{H}^\phi) - N^a (\mathcal{C}_a^G + \mathcal{C}_a^\phi) \right],
\]
up to surface terms, which do not concern us here. Therefore in the dust time gauge the diffeomorphism constraint reduces to that with only the gravity and scalar contributions, with physical Hamiltonian

$$\mathcal{H}_P = \int d^3 x \left( \mathcal{H}_G + \mathcal{H}_\phi \right).$$

The corresponding spacetime metric is

$$ds^2 = -dt^2 + (dx^a + N^a dt)(dx^b + N^b dt)q_{ab},$$

(18)

Let us note that numerous other matter time gauges are possible [22]. The advantage of the dust time gauge is the relative simplicity of the associated physical Hamiltonian.

A useful form of the symmetry reduction to homogeneous and isotropic cosmology is achieved with the parametrization

$$q_{ab} = \alpha a^{4/3}(t)e_{ab}, \quad \hat{\pi}^{ab} = \beta a^{-1/3} p_a(t)e^{ab}\sqrt{e},$$

(19)

where $\alpha$ and $\beta$ are constants and $e_{ab}$ is the flat 3–metric. This form is useful because the gravitational kinetic term in the physical hamiltonian becomes purely quadratic in $p_a$; $\alpha$ and $\beta$ are fixed by the conditions that the symplectic form $\pi^{ab}\hat{q}_{ab} \rightarrow p_a\dot{a}$, and the coefficient of the $p_a^2$ is unity. Furthermore, with this reduction the phase space is $\mathbb{R}^2$, and the spacetime metric is $ds^2 = -dt^2 + a^4(t)e_{ab}dx^a dx^b$. The physical Hamiltonian becomes

$$\mathcal{H}_P = -p_a^2 + \frac{p_\phi^2}{a^2},$$

(20)

after a rescaling of $p_\phi$. The negative sign in the gravitational kinetic term is of course expected since the DeWitt metric in the hamiltonian constraint of GR is not positive definite.

To summarize the steps so far, we derived the canonical theory of the action (4) in the dust time gauge, and then reduced to flat homogeneous and isotropic cosmology to arrive at (20); this physical Hamiltonian describes the coupled dynamics of the scale factor and scalar field in the dust time gauge.

Quantization and evolution. Standard quantization on the Hilbert space $L^2(\mathbb{R}) \otimes L^2(\mathbb{R})$ for the gravitational and scalar components leads to the Hamiltonian operator

$$\hat{\mathcal{H}} = \frac{\partial^2}{\partial a^2} - \frac{1}{a^2} \frac{\partial^2}{\partial \phi^2},$$

(21)

It is readily verified that the Hamiltonian is self-adjoint. Our focus is the time dependent Schrodinger equation. Although this equation is separable, for our purposes, it is convenient to solve it numerically for a range of initial states. The numerical method we use is an adaptation of the so-called Alternating Direction Implicit (ADI) scheme (see eg. [23]). With the discretization $\psi(a, \phi, t) \rightarrow U^*_{ni}$ where $n$ is the time step and $i, j$ the discrete $y, \phi$ grid, the ADI method divides a single time step evolution into two the implicit steps $n \rightarrow n^* \rightarrow n + 1$

$$U^* = U^n + \frac{\Delta t}{2} \left( \delta^2 a U^* - \frac{1}{a^2} \delta^2 \phi U^n \right),$$

$$U^{n+1} = U^* + \frac{\Delta t}{2} \left( \delta^2 a U^* - \frac{1}{a^2} \delta^2 \phi U^{n+1} \right),$$

(22)

where $\delta^2$ is a finite differencing of the second derivative. This evolution method preserves unitarity to a high degree.

Results. We computed the evolved wave function, partially traced density matrix, and entanglement entropy at each time step, for a variety of initial data using two different codes (written in MATLAB and Python). The variables used are dimensionless, scaled by the appropriate Planck units. The discretization grid used is $\Delta t = 10^{-5}$, and $\Delta a = \Delta \phi = 10^{-2}$. We performed calculations for the following classes of initial states, parametrized by $(\sigma, \phi_0, a_0, p_\phi^0, p_a^0)$: product states

![Image](image_url)

FIG. 1. Evolution of “multiverse” initial data, a linear combination of states of the type (23) where the scalar field momenta are of opposite sign. The lower frame demonstrates conservation of probability.
We have shown that in FRW quantum cosmology the scale factor and volume grow, the “effective coupling constant” $1/\alpha^2$ in the Hamiltonian (21) decreases rapidly to zero. This results in a dynamical decoupling of the scalar kinetic and gravity degrees of freedom. This in turn locks the wave function into a compact wave function. The lower frame shows the accuracy to which probability is conserved by our numerical scheme. These results are typical of the type of evolutions we observe. Evolution beyond the time indicated in these frames is similar, but with a further spreading of the wave function. The values of the initial data parameters correspond to Hubble parameters and scalar energy densities of order the Planck scale.

Fig. 2 shows the evolution of the scalar-geometry entanglement entropy as a function of dust time. Saturation of entropy is evident for each type of data. These plots are a typical subset of the type of evolution we see. We find no data for which saturation does not occur. There is an intuitive understanding of this result. As the scale factor and volume grow, the “effective coupling constant” $1/\alpha^2$ in the Hamiltonian (21) decreases rapidly to zero. This results in a dynamical decoupling of the scalar kinetic and gravity degrees of freedom. This in turn locks in the entropy gain achieved during the early evolution. As we are working in Planck units, it is evident that this occurs very quickly.

\[ \psi_0(a, \phi) = N a^2 \exp \left[ -\left( (\phi - \phi_0) + (a - a_0) \right)^2 / a^2 \right] 
\quad - a^2 \left( (\phi - \phi_0) - (a - a_0) \right)^2 
\quad + i \phi p_0^a + i a p_a^0 \right]. \]  
\[ \frac{\langle \psi | \hat{H} | \psi \rangle}{\alpha^2} \]

Our results appear in Figs. 1 to 3. Fig 1 shows a typical evolution of an MV state ($|\psi|^2$), where the initial wave function is a linear combination of two components of type (23); the upper frames show snapshots of the evolution of $|\psi|^2$. The form of the evolved wave function is curious; we see that the separated dots merge into a more compact wave function. The lower frame shows the accuracy to which probability is conserved by our numerical scheme. These results are typical of the type of evolutions we observe. Evolution beyond the time indicated in these frames is similar, but with a further spreading of the wave function. The values of the initial data parameters correspond to Hubble parameters and scalar energy densities of order the Planck scale.

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\[ \langle \psi | \hat{H} | \psi \rangle \]

Last, Fig. 3 gives plots of the saturation value of the entropy vs. expectation value of the Hamiltonian $\langle \hat{H} \rangle$ in the initial state for a variety of data; since the physical Hamiltonian is time independent, this expectation value is conserved. The linear relationship is evident, with slope (“inverse temperature”) dependent on the initial scale factor momentum $p_0^a$. 

\[ S_{\text{ent}}^\psi = \gamma \langle \psi | \hat{H} | \psi \rangle. \]

This equation represents a potential “First Law” for matter-geometry entanglement in quantum gravity. Also of note in Fig. 3 is the triple intersection of the three lines. It is not clear to us if this is significant, and whether it occurs for other types of data.

Discussion

We have shown that in FRW quantum cosmology with dust and scalar field, the scalar-geometry entanglement entropy exhibits remarkable features: a rapid increase followed by saturation, and a First Law. In deriving these results we made a number of assumptions.

The first is the selection of reduced phase space quantization, with a specific choice of clock. In contrast, in the “timeless” Dirac quantization approach, physical states of the Universe are fixed once and for all, and thus matter-geometry entanglement is frozen at the outset; this approach to quantum gravity yields a semiclassical “clock” only under certain assumptions, which include a late time product state ansatz for solutions of the Wheeler-DeWitt equation (see eg. [7]). Therefore in this “emergent” time approach there is no possibility of exploring entanglement entropy evolution in the deep quantum regime. Secondly, even within reduced phase space quantization, other clocks, such as volume time, are possible. However, volume time, like most others, leads to time dependent physical Hamiltonians. Dust time appears to be unique in yielding a time independent Hamiltonian. Ultimately such questions are connected to the problem of time in quantum gravity.

We studied two classes data: Gaussian, squeezed Gaussian initial data, and their “multiverse” linear combina-
tions. While this is a limitation, these are the simplest for initial investigations, and also provide a natural “Universe particle” interpretation; (similar data is used for example in Loop Quantum Cosmology [14]).

The numerically derived First Law (25) does not appear to have any obvious statistical mechanics explanation. $S_{\text{ent}}$ and $E$ are not macroscopic order parameters unless wave functions are viewed as providing ensemble averages. If this is assumed to be the case, each line in Fig. 3 would correspond to a system in equilibrium at a “temperature” $1/\gamma$ that depends on the initial Hubble parameter (a function of $p_0$).

Our results open several possibilities for further work. These include studying larger classes of initial data, and going beyond FRW to Bianchi cosmologies. The latter have been studied classically in dust time gauge [24], and would provide a richer arena for studying entanglement between between different scale factors, as well as with scalar fields. Of most interest would be the gravity-dust-scalar theory in spherical symmetry since this contains black hole solutions. This is of obvious relevance for black hole entropy and the “information loss problem;” that quantum gravity causes matter-gravity entanglement in such systems has been shown but not computed [25].

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