Quantum thermodynamics of de Sitter space

Robert Alicki,[1, *] Gabriela Barenboim,[2, †] and Alejandro Jenkins[1, 3, ‡]

[1]*International Centre for Theory of Quantum Technologies (ICTQT), University of Gdańsk, 80-308, Gdańsk, Poland*
[2]*Departament de Física Teòrica and IFIC, Universitat de València-CSIC, E-46100, Burjassot, Spain*
[3]*Laboratorio de Física Teórica y Computacional, Escuela de Física,*
Universidad de Costa Rica, 11501-2060, San José, Costa Rica
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We consider the local physics of an open quantum system embedded in an expanding three-dimensional space $\mathbf{x}$, evolving in cosmological time t, weakly coupled to massless quantum fields. We derive the corresponding Markovian master equation for the system's non-unitary evolution and show that, for a de Sitter (dS) space with Hubble parameter $h = $ const., the background fields act as a physical heat bath with temperature $T_{\mathrm{dS}} = h/2\pi$. The energy density of this bath obeys the Stefan-Boltzmann law $\rho_{\mathrm{dS}} \propto h^4$. We comment on how these results clarify the thermodynamics of dS space and support previous arguments for its instability in the infrared. The cosmological implications are considered in a accompanying letter [14].

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*Electronic address: robert.alicki@ug.edu.pl
†Electronic address: gabriela.barenboim@uv.es
‡Electronic address: alejandro.jenkins@ug.edu.pl

I. INTRODUCTION

According to Einstein's theory of General Relativity (GR), the size of our Universe is a dynamical quantity. The space-time geometry of a homogenous, isotropic, and Euclidean Universe can be described by the Friedmann-Lemaître-Robertson-Walker (FLRW) metric

$$ds^2 = -dt^2 + a^2(t)\, d\mathbf{x}^2, \tag{1}$$

where $(t, \mathbf{x}) = (t, x, y, z)$ are the space-time coordinates in the "cosmic rest frame" and $a(t) > 0$ is the scale factor that characterizes the size of the Universe. In terms of the Hubble parameter

$$h(t) \equiv \frac{\dot{a}(t)}{a(t)} \tag{2}$$

(where the dot indicates derivation with respect to time t) the GR field equations for the FLRW metric of Eq. (1) give us the first Friedmann equation

$$h^2 = \frac{8\pi\rho}{3}, \tag{3}$$

where $\rho(t)$ is the energy density of the Universe as a function of cosmological time. According to the second Friedmann equation,

$$\dot{h} = -\frac{3}{2}h^2 - 4\pi p, \tag{4}$$

where p is the pressure of the "cosmological fluid" with energy density ρ. Equations (3) and (4) imply the condition of covariant energy-momentum conservation:

$$\dot{\rho} = -3h(\rho + p). \tag{5}$$

In terms of the equation of state parameter $w \equiv p/\rho$, Eqs. (3) and (5) imply that h is constant if and only if $w = -1$. Throughout this article we work in Planck units, such that $G = M_{\mathrm{Pl}}^{-2} = \hbar = k_B = c = 1$.

Hubble's astronomical observations in 1929 implied an expanding Universe ($\dot{a} > 0$) [1]. This must have consequences for local physics. Already in 1939, Schrödinger argued that an accelerated expansion ($\ddot{a} > 0$) should be accompanied by what he called "alarming phenomena" of particle production or annihilation [2]. He drew this conclusion from the fact that such expansion mixes the positive and negative frequency terms in the Fourier expansion of a free relativistic field and, if the field is quantized, these terms are associated with production and annihilation of particles. The question of "cosmological particle production" has remained contentious in theoretical physics because of the ambiguity about the choice of vacuum state and the associated definition of particle number (see, e.g., [3] and references thererin).

In 1977, Gibbons and Hawking found that "an observer moving on a timelike geodesic in de Sitter space [i.e., with $h = \mathrm{const.}$] will detect thermal radiation" [4]. They interpreted the temperature of this radiation, $T_{\mathrm{dS}} = h/2\pi$, as resulting from the presence of an event horizon in de Sitter (dS) space, similar to the horizon of the Schwarzschild solution that leads to Hawking radiation from a black hole.

The Hawking temperature for a black hole of mass M is $T_H = 1/(8\pi M)$. The total energy of a black hole can be identified with its mass M, so that the first law of thermodynamics takes the form

$$dM = T_H dS + \Omega dJ + \Phi dQ, \tag{6}$$

where S is the black-hole entropy, J its angular momentum, Q its charge, Ω its angular velocity, and Φ its electrostatic potential at the horizon. This allows us to relate the Hawking temperature of the black hole to its entropy. Assuming that $S = 0$ for $M = 0$, Eq. (6) implies that $S = 4\pi M^2 = A_H/4$, where A_H is the area of black hole's event horizon. This approach, however, does not work for dS space, which has no extensive variable to play the role of M in Eq. (6) [5]. If we take the dS entropy to be proportional to the surface area of the event horizon in the same way as the black-hole entropy, we get $S_{\mathrm{dS}} = \pi/h^2$, which diverges in the Minkowski limit ($h \to 0$) in which the horizon disappears. How to interpret T_{dS} within a consistent thermodynamics for dS space remains contentious in high-energy theoretical physics: see, e.g., [6, 7] and references therein.

In 1981, Guth proposed that a short-lived dS phase in the early Universe could solve the horizon and flatness problems in cosmology [8]. This idea, which Guth called "inflation", soon became a pillar of modern cosmology, especially after it was shown that it could also account for the primordial density perturbations that seeded the subsequent formation of galaxies; see, e.g., [9] and references therein. However, despite the acceptance of inflation as a general paradigm, none of the many detailed models that have been proposed to implement it have thus far been generally regarded as wholly satisfactory. The main difficulties that any model of inflation faces are:

(a) to account for the very special (i.e., low-entropy) initial state of the Universe before inflation,

(b) to explain why inflation ended abruptly after the scale factor of the Universe had increased by $\gtrsim e^{60}$ ("60 e-folds"),

(c) to explain how the energy that drove inflation was converted into thermal radiation, generating the observed entropy of our Universe, and

(d) to explain why accelerated expansion re-started long after the end of inflation, at a far slower rate of exponential growth [10, 11].

In this article we study the thermodynamics of dS space using analytical techniques based on the Markovian master equation (MME) for an open quantum system (also known as the "GKLS equation" or the "Lindblad equation") [12, 13]. Taking such a system to be weakly coupled to a background massless quantum field and working in the cosmic rest frame for dS space, we find that the system equilibrates to a population distribution with temperature $T_{\mathrm{dS}} = h/2\pi$, consistent with the result of [4]. The authors of [4] concluded, based on the dS isometries, that any other observer moving along a timelike geodesic would also measure T_{dS}. We find, however, that this temperature is only well defined in the cosmic rest frame, in which the background acts as a *physical* heat bath whose energy density obeys the Stefan-Boltzmann law $\rho_{\mathrm{dS}} \propto T_{\mathrm{dS}}^4$.

In an accompanying letter [14], we combine this result with the Friedmann equations of classical GR and find that the dS phase ends abruptly because of the irreversible transfer of energy from the background ρ_{dS} into ordinary particles. This provides a graceful exit to inflation without the need to invoke any inflaton potential. Thermal particle production during inflation, with a black-body spectrum given by T_{dS} (rather than vacuum fluctuations) can explain the presence of adiabatic, Gaussian, and approximately scale-invariant primordial perturbations that seed the subsequent formation of structure in the Universe.

Various authors have already argued that dS space is unstable in the infrared (IR) and that such an instability may explain how inflation ends and why the cosmological constant is currently so small compared to the natural scale M_{Pl}^4; see, e.g., [15–23] (this list is far from exhaustive). However, our limited understanding of the thermodynamics of dS space has obscured the logical relations among these various arguments and prevented any of them from being widely accepted as decisive. This work seeks to apply to that problem the analytical methods of open quantum systems and quantum thermodynamics. Such an approach has, thus far, been used mostly in quantum optics (for an introduction to quantum thermodynamics and its history, see [24]). The resulting formulation of the local dynamics in dS space is not generally covariant. This is a feature and not a bug of our approach. It is well established —though perhaps not very widely appreciated— that thermodynamic quantities are necessarily *not* covariant in quantum physics [25] (see also the discussion in the Appendix). In the case of dS, it has been shown explicitly that a finite entropy breaks the classical space-time symmetries [26].

The combined results of this article and of [14] have direct relevance to points (b) and (c) in the above list of difficulties faced by theories of inflation. Our analysis may also have something to contribute to point (a), as we comment upon briefly in Sec. IV C, but this point remains speculative. We have nothing to contribute on point (d) (the "small cosmological constant problem"), except to the extent that our results could be combined with further efforts of model building aimed specifically at accounting for the current phase of slowly accelerating expansion.

II. LOCAL PHYSICS IN EXPANDING SPACE

We seek to describe the irreversible dynamics of an open quantum system embedded in an expanding three-dimensional space $\mathbf{x} = (x, y, z)$ and evolving in cosmological time t. If the system in static space is characterized by the Hamiltonian $\hat{H}$, then its dynamics in an expanding space can be expressed by the modified Hamiltonian

$$\hat{H}_D(t) = \hat{H} + h(t)\hat{D}, \tag{7}$$

where $\hat{D}$ is the spatial dilation operator and $h(t)$ is the Hubble parameter defined in Eq. (2). This separation of $\hat{H}$ is valid if we may neglect the back-reaction of the dynamics of the system on the space-time, and it is therefore equivalent to the fundamental approximation made in calculations of quantum fields in curved space-time (see, e.g., [27, 28] and references thererin). In the accompanying letter [14] we include the back-reaction via an adiabatic approximation, by taking $h(t)$ from the classical Friedmann equations (3) and (4), which is consistent with the usual approach in cosmology.

This formulation is not coordinate invariant, but it will allow us to apply the analytical machinery of quantum thermodynamics in a straightforward way. Moreover, in cosmology we are primarily interested in how the dynamics

appears to an observer in the cosmic rest frame of Eq. (1). The formulation of Eq. (7) is analogous to that of previous work in which the quantum thermodynamics of moving baths (including black-hole superradiance) was studied using an effective Hamiltonian shifted by rotation [29], with the important difference that in that case $\hat{H}$ was taken to commute with the generator of rotations $\hat{L}_z$, whereas now we do not take $\hat{H}$ to commute with $\hat{D}$.

For a wave function $\psi(\mathbf{x})$ the operator $\hat{D}$ is defined by

$$\left[e^{-i\lambda\hat{D}}\psi\right](\mathbf{x}) = e^{-\frac{3}{2}\lambda}\psi\left(e^{-\lambda}\mathbf{x}\right), \tag{8}$$

and hence

$$\hat{D} = \frac{1}{2}\left(\hat{\mathbf{x}}\cdot\hat{\mathbf{p}} + \hat{\mathbf{p}}\cdot\hat{\mathbf{x}}\right), \tag{9}$$

which is a particular case of the "squeeze operator". The Hamiltonian of Eq. (7) for a single non-relativistic particle is

$$\hat{H}_D(\hat{\mathbf{x}}, \hat{\mathbf{p}}; t) = \frac{\hat{\mathbf{p}}^2}{2m} + U(\hat{\mathbf{x}}) + \frac{1}{2}h(t)\left(\hat{\mathbf{x}}\cdot\hat{\mathbf{p}} + \hat{\mathbf{x}}\cdot\hat{\mathbf{p}}.\right) \tag{10}$$

Under the unitary transformations $\hat{\mathbf{x}} \mapsto \hat{\mathbf{x}}$ and $\hat{\mathbf{p}} \mapsto \hat{\mathbf{p}} + hm\hat{\mathbf{x}}$ this becomes.

$$\hat{H}'_D(\hat{\mathbf{x}}, \hat{\mathbf{p}}; t) = \frac{\hat{\mathbf{p}}^2}{2m} + U(\hat{\mathbf{x}}) - \frac{1}{2}mh^2(t)\hat{\mathbf{x}}^2 \tag{11}$$

As a check that Eq. (7) gives the correct local physics in an expanding Universe, consider a two-body system governed by the classical version of Eqs. (7) and (9):

$$H(\mathbf{x}, \mathbf{p}; t) = \frac{\mathbf{p}_A^2}{2m_A} + \frac{\mathbf{p}_B^2}{2m_B} + U(\mathbf{x}_A - \mathbf{x}_B) + h(t)\left(\mathbf{x}_A\cdot\mathbf{p}_A + \mathbf{x}_B\cdot\mathbf{p}_B\right). \tag{12}$$

Using the index $K = A, B$, the corresponding Hamiltonian equations can be written as

$$\dot{\mathbf{x}}_K = \frac{\partial H}{\partial \mathbf{p}_K} = \frac{\mathbf{p}_K}{m_K} + h(t)\mathbf{x}_K, \quad \dot{\mathbf{p}}_K = -\frac{\partial H}{\partial \mathbf{x}_K} = -\frac{\partial}{\partial \mathbf{x}_K}U(\mathbf{x}_A - \mathbf{x}_B) - h(t)\mathbf{p}_K. \tag{13}$$

From Eq. (13) one obtains the Newtonian equations of motion

$$m_K\ddot{\mathbf{x}}_K = -\frac{\partial}{\partial \mathbf{x}_K}U(\mathbf{x}_A - \mathbf{x}_B) + m_K\left[h^2(t) + \dot{h}(t)\right]\mathbf{x}_K. \tag{14}$$

Introducing the center of mass coordinate $\mathbf{X} = M^{-1}(m_A\mathbf{x}_A + m_B\mathbf{x}_B)$, $M = m_A + m_B$, and the relative position $\mathbf{x} = \mathbf{x}_A - \mathbf{x}_B$ this becomes

$$\ddot{\mathbf{X}} = \left[h^2(t) + \dot{h}(t)\right]\mathbf{X}, \tag{15}$$

$$\ddot{\mathbf{x}} = -\frac{1}{\mu}\frac{\partial}{\partial \mathbf{x}}U(\mathbf{x}) + \left[h^2(t) + \dot{h}(t)\right]\mathbf{x}, \quad \mu = \frac{m_Am_B}{m_A + m_B}. \tag{16}$$

For $h = \text{const.}$ (dS space) the contribution from expansion to Eq. (16) takes the form of a negative (unstable) harmonic potential. This agrees with the "all or nothing" picture presented in [31, 32]: a tightly bound classical system will, after some initial disturbance of its orbit, evolve with bounded $|\mathbf{x}|$, unaffected by the continuing expansion of space, while the center of mass follows the Universe's expansion.

Note that there is an obvious canonical quantization of the system described by Eq. (14). For a tightly bound system we expect that bound states are only slightly perturbed by the dilation. However, none of them will be eigenvectors of the total Hamiltonian with the dilation term. Instead, they will be resonances that decay by tunneling through the potential barrier. The lifetime of such a resonance can be very long if the system is tightly bound compared to the rate of expansion, but this already suggests that quantum systems in dS space are unstable in the infrared. This is a crucial issue that we shall return to in Sec. IV C in light of the analytical results of quantum thermodynamics.

III.   MARKOVIAN MASTER EQUATION

The MME has been applied previously to early-Universe cosmology: see, e.g., [33–38] and references therein. As far as we know, however, it has only been used to describe decoherence effects and not the thermal processes that concern us here. In particular, our objective is to study the thermodynamics of dS space, based on the MME for an open quantum system that is embedded in an expanding space and weakly coupled to a background massless quantum field. Since this is a new application of an approach to thermal physics that has not been widely used in high-energy physics or cosmology, in this section we define the main mathematical objects used in the rest of this article, based on a concrete example: a simple harmonic oscillator weakly coupled to a thermal bath of bosons. The general analytical methods and results from the theory of open quantum systems relevant to the present discussion are briefly reviewed in the Appendix. For further details, see [39] and references therein.

A.   Example: Harmonic oscillator in a bosonic bath

Let us begin by reviewing the results of the MME applied to a harmonic oscillator weakly coupled to a bosonic bath. The purpose of this exercise is to introduce the relevant concepts and analytical techniques in an intuitive and physically well motivated context. Those same concepts and techniques will then be applied in Sec. IV to the thermodynamics of dS space.

The bare Hamiltonian of the harmonic oscillator reads

$$\hat{H}_0 = \omega_0 \hat{b}^\dagger \hat{b}, \quad \text{with} \quad \left[\hat{b}, \hat{b}^\dagger\right] = 1. \tag{17}$$

The thermal bath consists of noninteracting bosons with the dispersion law $\omega(\mathbf{k}) \geq 0$ and occupying an infinite three-dimensional space. The bath Hamiltonian,

$$\hat{H}_B = \int d^3k\, \omega(\mathbf{k}) \hat{a}^\dagger(\mathbf{k}) \hat{a}(\mathbf{k}), \tag{18}$$

is given in terms of annihilation and creations field operators satisfying the canonical commutation relation:

$$\left[\hat{a}(\mathbf{k}), \hat{a}^\dagger(\mathbf{k}')\right] = \delta^{(3)}(\mathbf{k} - \mathbf{k}'). \tag{19}$$

The density of states (per unit volume) at a given energy ω is

$$n(\omega) = \int \frac{d^3k}{(2\pi)^3} \delta[\omega - \omega(\mathbf{k})]. \tag{20}$$

The equilibrium state of a bosonic gas at the inverse temperature β is fully characterized by the second-order correlations

$$\left\langle \hat{a}^\dagger(\mathbf{k}) \hat{a}(\mathbf{k}') \right\rangle_\beta = \frac{1}{e^{\beta\omega(\mathbf{k})} - 1} \delta^{(3)}(\mathbf{k} - \mathbf{k}'), \tag{21}$$

where $\langle \cdots \rangle_\beta$ denotes the average with respect to equilibrium state with inverse temperature β. Note that here we have simply *assumed* that the bosons are in the thermal state characterized by Eq. (21).

The coupling of the harmonic oscillator to the bath is given by the interaction Hamiltonian

$$\hat{H}_{\text{int}} = \lambda \left(\hat{b} + \hat{b}^\dagger\right) \otimes \hat{\phi}_\Lambda(0), \tag{22}$$

Here, the harmonic oscillator is localized at the origin of the coordinate system and locally coupled to the field at that point. To obtain a mathematically well-defined Hamiltonian we regularize the quantum field at the point using an ultraviolet cut-off parameter Λ, such that

$$\hat{\phi}_\Lambda(0) = \int \frac{d^3k}{\sqrt{2\omega(\mathbf{k})}} e^{-\omega(\mathbf{k})/\Lambda} \left[\hat{a}(\mathbf{k}) + \hat{a}^\dagger(\mathbf{k})\right]. \tag{23}$$

We then apply the standard derivation of the MME for the density matrix $\hat{\rho}(t)$ for the mixed state of the harmonic oscillator, averaging over the bath's degrees of freedom in its equilibrium state. The resulting MME is a special case of the general form given in the Appendix. In terms of the renormalized Hamiltonian $\hat{H}$, this is

$$\frac{d}{dt}\hat{\rho}(t) = -i\left[\hat{H}, \hat{\rho}(t)\right] + \frac{1}{2}\left(\gamma_\downarrow \left(\left[\hat{b}, \hat{\rho}(t)\hat{b}^\dagger\right] + \left[\hat{b}\hat{\rho}(t), \hat{b}^\dagger\right]\right) + \gamma_\uparrow \left(\left[\hat{b}^\dagger, \hat{\rho}(t)\hat{b}\right] + \left[\hat{b}^\dagger\hat{\rho}(t), \hat{b}\right]\right)\right) \tag{24}$$

with damping and pumping rates

$$\gamma_\downarrow = \lambda^2 \tilde{G}(\omega) \quad \text{and} \quad \gamma_\uparrow = \lambda^2 \tilde{G}(-\omega), \tag{25}$$

expressed in terms of the *spectral density* $\tilde{G}(\omega)$ for the renormalized frequencies ω. This spectral density is given by the Fourier transform of the *bath correlation function* $G(t)$ (see Appendix).

B. Spectral density function

In this case we have

$$\tilde{G}(\omega) = \lim_{\Lambda \to \infty} \tilde{G}_\Lambda(\omega) = \lim_{\Lambda \to \infty} \int_{-\infty}^{+\infty} dt \, e^{i\omega t} G_\Lambda(t) = \lim_{\Lambda \to \infty} \int_{-\infty}^{+\infty} dt \, e^{i\omega t} \left\langle \hat{\phi}_\Lambda(t) \hat{\phi}_\Lambda(0) \right\rangle_\beta$$

$$= \lim_{\Lambda \to \infty} \int_{-\infty}^{+\infty} dt \, e^{i\omega t} \left\langle e^{i\hat{H}_B t} \hat{\phi}_\Lambda(0) e^{-i\hat{H}_B t} \hat{\phi}_\Lambda(0) \right\rangle_\beta$$

$$= \lim_{\Lambda \to \infty} \int d^3k \int_{-\infty}^{+\infty} dt \, e^{i\omega t} \frac{e^{-2\omega(\mathbf{k})/\Lambda}}{2\omega(\mathbf{k})} \left\{ \left\langle \hat{a}(\mathbf{k}) \hat{a}^\dagger(\mathbf{k}) \right\rangle_\beta e^{-i\omega(\mathbf{k})t} + \left\langle \hat{a}^\dagger(\mathbf{k}) \hat{a}(\mathbf{k}) \right\rangle_\beta e^{i\omega(\mathbf{k})t} \right\}$$

$$= \pi \int d^3k \frac{1}{\omega} \left\{ \delta[\omega - \omega(\mathbf{k})] \frac{1}{1 - e^{-\beta\omega}} + \delta[\omega + \omega(\mathbf{k})] \frac{1}{e^{\beta\omega} - 1} \right\}. \tag{26}$$

Using Eq. (20) one obtains

$$\tilde{G}(\omega) = \frac{8\pi^4 n(|\omega|)}{\omega(1 - e^{-\beta\omega})}. \tag{27}$$

One can check the Kubo-Martin-Schwinger (KMS) property of the spectral density (see Appendix)

$$\tilde{G}(-\omega) = e^{-\beta\omega} \tilde{G}(\omega), \tag{28}$$

which implies that the Gibbs state $\hat{\rho}_\beta = Z^{-1} e^{-\beta\hat{H}}$ is an equilibrium state for the harmonic oscillator and, moreover, that any initial state relaxes to $\hat{\rho}_\beta$. The harmonic oscillator can therefore be treated as a thermometer that measures the temperature of the bosonic bath.

C. Noise spectra

The bosonic heat bath at equilibrium is a source of thermal/quantum noise characterized by two different spectra associated with $\tilde{G}(\omega)$. The first one is the *field fluctuation spectrum* $\mathcal{P}(\omega)$ defined as

$$\int_0^\infty d\omega \, \mathcal{P}(\omega) = \lim_{\Lambda \to \infty} \langle \hat{\phi}_\Lambda^2 \rangle_\beta. \tag{29}$$

This average can be written as

$$\langle \hat{\phi}_\Lambda^2 \rangle_\beta = \int_0^\infty d\omega \int d^3k \, \delta[\omega - \omega(\mathbf{k})] e^{-2\omega(\mathbf{k})/\Lambda} \frac{\left\langle \hat{a}^\dagger(\mathbf{k}) \hat{a}(\mathbf{k}) + \hat{a}(\mathbf{k}) \hat{a}^\dagger(\mathbf{k}) \right\rangle_\beta}{2\omega(\mathbf{k})}$$

$$= (2\pi)^3 \int_0^\infty d\omega \frac{e^{-2\omega/\Lambda}}{\omega} n(\omega) \left(\frac{1}{e^{\beta\omega} - 1} + \frac{1}{2} \right). \tag{30}$$

This can be decomposed into thermal and vacuum contributions:

$$\mathcal{P}(\omega) = \mathcal{P}_{\text{th}}(\omega) + \mathcal{P}_{\text{vac}}(\omega), \quad \mathcal{P}_{\text{th}}(\omega) = (2\pi)^3 \frac{n(\omega)}{\omega(e^{\beta\omega} - 1)}, \quad \mathcal{P}_{\text{vac}}(\omega) = 4\pi^3 \frac{n(\omega)}{\omega}. \tag{31}$$

The $\mathcal{P}_{\text{vac}}$ can be renormalized to zero by using normal ordering for the powers of field, as is usually done in statistical mechanics.

The second spectrum associated with $\tilde{G}(\omega)$ is the *energy density spectrum* $\mathcal{U}(\omega)$, given by

$$\mathcal{U}(\omega) = \frac{n(\omega)\,\omega}{e^{\beta\omega} - 1}. \tag{32}$$

This coincides with the Planck distribution (per single polarization) for massless scalar bosons with $\omega(\mathbf{k}) = |\mathbf{k}|$ and density of states

$$n(\omega) = \frac{\omega^2}{2\pi^2}. \tag{33}$$

The two spectra are related by

$$\mathcal{P}_{\mathrm{th}}(\omega) = 2\pi\tilde{G}(-\omega) \quad \text{and} \quad \mathcal{U}(\omega) = \frac{\omega^2}{(2\pi)^3}\mathcal{P}_{\mathrm{th}}(\omega) = \frac{\omega^2}{(2\pi)^2}\tilde{G}(-\omega). \tag{34}$$

IV. QUANTUM FIELD IN EXPANDING UNIVERSE

It should be clear from the discussion in Sec. III that our main task, in order to describe the thermodynamics of dS space analytically, is to find the corresponding spectral density $\tilde{G}(\omega)$, which is given by the Fourier transform of the bath correlation function $G(t)$ [see Eq. (26)]. To obtain $G(t)$ we need to know how the operator $\hat{\phi}_\Lambda(0)$ of Eq. (23) evolves in cosmological time t, for an expanding space $\mathbf{x}$ characterized by the Hubble parameter $h(t)$. It is important to emphasize that, unlike in Sec. III, here we will not assume any thermal state. Instead, we will show that in dS space the quantum vacuum acts as a thermal bath, and we will compute its temperature and noise spectra. Our treatment is similar in spirit to the derivation of the Unruh effect presented in [40].

A. Time-evolution operator

Let us consider a scalar field described in the cosmic rest frame at some initial cosmological time (say, $t_0 = 0$) by annihilation and creation operators $\hat{a}(\mathbf{k}), \hat{a}^\dagger(\mathbf{k})$ satisfying the commutation relations of Eq. (19). The reference state of the field is the vacuum $|\Omega\rangle$ satisfying $\hat{a}(\mathbf{k})|\Omega\rangle = 0$, which is consistent with the Bunch-Davies condition for the dS vacuum [41]. The effects of the expansion of space are accounted for by adding a time-dependent dilation generator to the free Hamiltonian, as in Eq. (7). For a single massless scalar boson we have

$$\hat{H}_D(t) = \hat{H} + h(t)\hat{D}, \quad \hat{H} = |\mathbf{k}|, \quad \hat{D} = i\left(\mathbf{k}\frac{\partial}{\partial\mathbf{k}} + i\frac{3}{2}\right). \tag{35}$$

In order to solve the corresponding Schrödinger evolution equation we use the commutation relation

$$\left[\hat{D}, \hat{H}\right] = i\hat{H}. \tag{36}$$

By the Baker-Hausdorff lemma, this implies that

$$e^{-i\alpha\hat{D}}\hat{H}e^{i\alpha\hat{D}} = e^\alpha\hat{H}. \tag{37}$$

The time-evolution operator for a single boson can be written as

$$\hat{U}(t) = \mathbf{T}\exp\left[-i\int_0^t ds\,\left(\hat{H} + h(s)\hat{D}\right)\right] = e^{-i\nu(t)\hat{D}}e^{-i\tau(t)\hat{H}}. \tag{38}$$

The time-ordering symbol $\mathbf{T}$ is needed if $h(t)$ is not constant, since then

$$[\hat{H}_D(t_1), \hat{H}_D(t_2)] = i[h(t_1) - h(t_2)]\hat{H} \neq 0 \quad \text{for} \quad t_1 \neq t_2. \tag{39}$$

To show that $\hat{U}(t)$ does indeed take the form given in Eq. (38), we compute its derivative in time:

$$\hat{U}'(t) = -i\nu'(t)\hat{D}\hat{U}(t) + e^{-i\nu(t)\hat{D}}\left(-i\tau'(t)\hat{H}\right)e^{-i\tau(t)\hat{H}} = -i\left[\nu'(t)\hat{D} + \tau'(t)e^{-i\nu(t)\hat{D}}\hat{H}e^{i\nu(t)\hat{D}}\right]\hat{U}(t). \tag{40}$$

Using Eq. (37), we conclude that, as long as

$$\nu(t) = \int_0^t ds\, h(s) \quad \text{and} \quad \tau(t) = \int_0^t ds\, e^{-\nu(s)}, \tag{41}$$

this $\hat{U}(t)$ obeys the Schrödinger equation

$$\hat{U}'(t) = -i\hat{H}_D(t)\,\hat{U}(t) \quad \text{for} \quad \hat{U}(0) = 1. \tag{42}$$

In particular, for constant h

$$\nu(t) = ht \quad \text{and} \quad \tau(t) = \frac{1 - e^{-ht}}{h}. \tag{43}$$

The evolution of a massless bosonic wavepacket in the expanding space can therefore be represented as the composition of the propagation in stationary space, albeit with slowed-down time $\tau(t)$ of Eq. (41) (called "conformal time" in the cosmological literature), and the dilation map. For a plane-wave mode with $\hat{H}|\mathbf{k}\rangle = |\mathbf{k}|\cdot|\mathbf{k}\rangle$, the condition $\tau(t)\cdot|\mathbf{k}| \ll 1$ implies that the time-evolution operator of Eq. (38) is completely dominated by the dilation $\exp\left[-i\nu(t)\hat{D}\right]$. This corresponds to the "freezing in" of modes with wavelengths larger than the causal horizon ("super-horizon modes") during inflation. Note that throughout this article we work in terms of the physical (rather than the comoving) momenta.

B. de Sitter vacuum as heat bath

We consider a dS universe in the vacuum state $|\Omega\rangle$ of the massless scalar field. The physics of this state can be tested by putting a localized system, such as the thermometer discussed Sec. III A, in contact with the background scalar field. The quantum noise acting on this system is fully characterized by the background field's second order correlation function, or by its Fourier transform [Eq. (26)]. In order to characterize the properties of the dS vacuum we compute the analog of the bath correlation function $G_\Lambda(t)$ that appeared in Eq. (26):

$$G_\Lambda^{dS}(t) = \langle\Omega|e^{i\hat{H}_{dS}t}\hat{\phi}_\Lambda(0)e^{-i\hat{H}_{dS}t}\hat{\phi}_\Lambda(0)|\Omega\rangle \tag{44}$$

where $\hat{\phi}_\Lambda(0)$ is given by Eq. (23) with $\omega(\mathbf{k}) = |\mathbf{k}|$, and $\hat{H}_{dS}$ is the second quantization (i.e., lifting to Fock space) of the single-boson Hamiltonian $\hat{H}_D$ in Eq. (35) for $h = \text{const}$. Then

$$G_\Lambda^{dS}(t) = \langle g_\Lambda|\hat{U}(t)|g_\Lambda\rangle, \tag{45}$$

where $\hat{U}(t)$ is given by Eqs. (38), (43), and the momentum representation of the wave function for g_Λ,

$$\tilde{\psi}(\mathbf{k}) = \langle\mathbf{k}|g_\Lambda\rangle = \frac{e^{-|\mathbf{k}|/\Lambda}}{\sqrt{2|\mathbf{k}|}}. \tag{46}$$

The corresponding wavefunction in position representation is:

$$\psi(\mathbf{x}) = \langle\mathbf{x}|g_\Lambda\rangle = \int d^3k\, \langle\mathbf{x}|\mathbf{k}\rangle\langle\mathbf{k}|g\rangle = \int \frac{d^3k}{(2\pi)^{3/2}} \frac{e^{-i\mathbf{k}\cdot\mathbf{x}}e^{-|\mathbf{k}|/\Lambda}}{\sqrt{2|\mathbf{k}|}}, \tag{47}$$

in the convention for the Fourier transform in which

$$\langle\mathbf{x}|\mathbf{k}\rangle = \frac{e^{-i\mathbf{k}\cdot\mathbf{x}}}{(2\pi)^{3/2}}. \tag{48}$$

In this case,

$$\langle\mathbf{x}|e^{-i\tau(t)\hat{H}}|g_\Lambda\rangle = \int d^3k\, \langle\mathbf{x}|e^{-i\tau(t)\hat{H}}|\mathbf{k}\rangle\langle\mathbf{k}|g_\Lambda\rangle = \int d^3k\, e^{-i|\mathbf{k}|\tau(t)}\langle\mathbf{x}|\mathbf{k}\rangle\langle\mathbf{k}|g\rangle = \int \frac{d^3k}{(2\pi)^{3/2}} \frac{e^{-i|\mathbf{k}|\tau(t)}e^{-i\mathbf{k}\cdot\mathbf{x}}e^{-|\mathbf{k}|/\Lambda}}{\sqrt{2|\mathbf{k}|}}. \tag{49}$$

Using Eq. (8) for the action of the dilation operator on the wavefunction, we have that

$$\langle \mathbf{x}|e^{i\nu(t)\hat{D}}|g_\Lambda\rangle = \left[e^{i\nu(t)\hat{D}}\psi\right](\mathbf{x}) = \frac{e^{\frac{3}{2}\nu(t)}}{(2\pi)^{3/2}}\int d^3k' \frac{e^{-|\mathbf{k}'|/\Lambda}}{\sqrt{2|\mathbf{k}'|}}e^{-i\mathbf{k}'\cdot\mathbf{x}e^{\nu(t)}}. \tag{50}$$

The bath correlation function of Eq. (45) can therefore be expressed as

$$G_\Lambda^{dS}(t) = \int d^3x\, \langle g_\Lambda|e^{-i\nu(t)\hat{D}}|\mathbf{x}\rangle\langle\mathbf{x}|e^{-i\tau(t)\hat{H}}|g_\Lambda\rangle = \frac{1}{(2\pi)^3}\int d^3x\, d^3k\, d^3k'\, e^{\frac{3}{2}\nu(t)}\frac{e^{-(|\mathbf{k}|+|\mathbf{k}'|)/\Lambda}}{2\sqrt{|\mathbf{k}|\cdot|\mathbf{k}'|}}e^{-i|\mathbf{k}|\tau(t)}e^{-i(\mathbf{k}-e^{\nu(t)}\mathbf{k}')\cdot\mathbf{x}}$$

$$= e^{\frac{3}{2}\nu(t)}\int d^3k\, d^3k'\, \frac{e^{-(|\mathbf{k}|+|\mathbf{k}'|)/\Lambda}}{2\sqrt{|\mathbf{k}|\cdot|\mathbf{k}'|}}e^{-i|\mathbf{k}|\tau(t)}\delta^{(3)}\left(\mathbf{k}-e^{\nu(t)}\mathbf{k}'\right) = e^{-\frac{3}{2}\nu(t)}\int d^3k\, \frac{e^{-\left(1+e^{-\nu(t)}\right)|\mathbf{k}|/\Lambda}}{2|\mathbf{k}|e^{-\nu(t)/2}}e^{-i|\mathbf{k}|\tau(t)}$$

$$= 2\pi e^{-\nu(t)}\int_0^\infty dr\, r\exp\left[-r\left(\frac{1+e^{-\nu(t)}}{\Lambda}+i\tau(t)\right)\right] = 2\pi e^{-\nu(t)}\left(\frac{1+e^{-\nu(t)}}{\Lambda}+i\tau(t)\right)^{-2}. \tag{51}$$

For constant h this becomes:

$$G_\Lambda^{dS}(t) = \frac{\pi}{2}\left(\frac{h\Lambda}{h\cosh\frac{ht}{2}+i\Lambda\sinh\frac{ht}{2}}\right)^2. \tag{52}$$

In the convention of Eq. (26), the corresponding spectral density is:

$$\tilde{G}_\Lambda^{dS}(\omega) = 2\pi^2\Lambda^2\frac{\omega}{h^2+\Lambda^2}\mathrm{csch}\left(\frac{\pi\omega}{h}\right)\exp\left[\frac{2\omega}{h}\arcsin\left(\frac{\Lambda}{\sqrt{h^2+\Lambda^2}}\right)\right]. \tag{53}$$

Note that $\tilde{G}_\Lambda^{dS}(\omega) > 0$, as required by Bochner's theorem (see also the discussion in the Appendix). The fact that this spectral density has support on $\omega < 0$ indicates a dynamical instability associated with particle production. We can compute the Boltzmann factor according to Eq. (28), which gives us

$$\beta = \frac{4}{h}\arcsin\left(\frac{\Lambda}{\sqrt{\Lambda^2+h^2}}\right). \tag{54}$$

In the limit $\Lambda\to\infty$, this gives the usual dS temperature

$$T_{\mathrm{dS}} = \frac{1}{\beta} = \frac{h}{2\pi}. \tag{55}$$

The dS spectral density is

$$\tilde{G}^{dS}(\omega) \equiv \lim_{\Lambda\to\infty}\tilde{G}_\Lambda^{dS}(\omega) = 2\pi^2\omega\,\mathrm{csch}\left(\frac{\omega}{2T_{\mathrm{dS}}}\right)e^{\omega/2T_{\mathrm{dS}}} = \frac{(2\pi)^2\omega}{1-e^{-\omega/T_{\mathrm{dS}}}}. \tag{56}$$

Comparing this to Eq. (27), we conclude that dS space acts as a thermal bath with density of states

$$n^{dS}(\omega) = \frac{\omega\tilde{G}^{dS}(\omega)\left(1-e^{-\omega/T_{\mathrm{dS}}}\right)}{8\pi^4} = \frac{\omega^2}{2\pi^2}, \tag{57}$$

as in Eq. (33).

The energy density of the dS bath obeys the Stefan-Boltzmann law:

$$\rho_{\mathrm{dS}} = g_f\int_0^\infty d\omega\,\mathcal{U}^{dS}(\omega) = g_f\int_0^\infty d\omega\,\frac{n^{dS}(\omega)\,\omega}{e^{\omega/T_{\mathrm{dS}}}-1} = \frac{g_f}{2\pi^2}\int_0^\infty\frac{d\omega\,\omega^3}{e^{\omega/T_{\mathrm{dS}}}-1} = \frac{g_f T_{\mathrm{dS}}^4}{2\pi^2}\int_0^\infty\frac{dx\,x^3}{e^x-1} = \frac{g_f\pi^2}{30}T_{\mathrm{dS}}^4, \tag{58}$$

where g_f denotes the number of degrees of freedom in the bath (which we have assumed to correspond to massless fields), and where we have used the energy density spectrum of Eq. (32) with the density of states of Eq. (57). In terms of the Hubble parameter,

$$\rho_{\mathrm{dS}} = \sigma h^4, \quad \text{for} \quad \sigma \equiv \frac{g_f}{480\pi^2}. \tag{59}$$

Note that, in line with the arguments of [25] for physical heat baths, only the observer in the cosmic rest frame will measure T_{dS}. Boosts with respect to this frame break the KMS condition of Eq. (28) due to Doppler shifts of the mode frequencies, so that the bath will not appear in equilibrium (the results of [29, 30], in which Doppler shifts were introduced by rotational motion, can be easily extended to linear motion). This is an important difference with the original results of Gibbons and Hawking [4], in which T_{dS} was interpreted as preserving the isometries of dS space. Polyakov has emphasized in [22] that the absence of such Doppler shifts prevents us from interpreting the result of [4] in terms of a physical heat bath.

We calculated $\tilde{G}^{dS}(\omega)$ and the associated thermal properties for a single background massless scalar field. In fact, all of the quantum fields present should be included in the calculation of the bath correlation function. Fortunately, it is not difficult to extend our results in that way, as long as h is large enough that the masses of the fields can be neglected. For fermions, the thermal power spectrum and the energy density spectrum [Eqs. (31) and (32)] become, respectively,

$$\mathcal{P}_{\mathrm{th}}(\omega) = (2\pi)^3 \frac{n(\omega)}{\omega(e^{\beta\omega} + 1)} \quad \text{and} \quad \mathcal{U}(\omega) = \frac{n(\omega)\,\omega}{e^{\beta\omega} + 1}. \tag{60}$$

For $\beta\omega \ll 1$, the contribution of fermions to the thermal power spectrum can therefore be neglected relative to the contribution from bosons. The fermion contribution to ρ_{dS} in Eq. (58) is weighed by a factor of

$$\int_0^\infty \frac{dx\,x^3}{e^x + 1} \Big/ \int_0^\infty \frac{dx\,x^3}{e^x - 1} = \frac{7}{8}, \tag{61}$$

as is well known in cosmology for the energy density of ordinary thermal radiation (see, e.g., sec. 3.3 in [42]).

C.   Infrared instability

The results of Sec. IV B were derived assuming $h = \mathrm{const}$. As long as the space-time geometry remains homogenous and isotropic, and if the change in h is very slow compared to the Planck-time scale that controls the gravitational microphysics, we may use Eq. (59) as an adiabatic relation between $h(t)$ and the heat bath's contribution $\rho_{\mathrm{dS}}(t)$ to the energy density of the early Universe. By including terms corresponding to this contribution in the Friedmann Eqs. (3) and (4), we can take into account the back-reaction of the heat bath on the space-time. This is done in the accompanying letter [14].

The bath with energy density ρ_{dS} can be considered as a cosmological fluid whose pressure p_{dS} obeys the equation of state $w_{\mathrm{dS}} = p_{\mathrm{dS}}/\rho_{\mathrm{dS}} = -1$. The bath must obey this equation of state because the energy density of Eq. (58) is not diluted by the expansion of the Universe, as per Eq. (5) (the increasing amount of energy in this fluid as the Universe expands is compensated by the negative energy of gravity). We may therefore write the total energy density of the Universe as

$$\rho = \rho_{\mathrm{dS}} + \rho_r = \sigma h^4 + \rho_r \tag{62}$$

and the total pressure as

$$p = p_{\mathrm{dS}} + p_r = -\sigma h^4 + w_r \rho_r. \tag{63}$$

By combining Eqs. (62) and (63) with the Friedmann equations, we show in [14] that —much like in a superheated liquid— a perturbation may trigger a spontaneous boiling, which in the cosmological case corresponds to the production of radiation with equation of state $w_r = p_r/\rho_r = 1/3$. This boiling relaxes the temperature, so that $h \to 0$. This leads us to conclude that dS space is, as previous of authors have argued on a variety of grounds, unstable in the IR. This picture gives us the main features of inflation without invoking any inflaton potential function, or even a coherent inflaton field.

In the case of boiling water, the microscopic details are complicated, but the process can be understood macroscopically with the aid of the laws of thermodynamics. A microscopic description of inflation would require a better understanding of quantum gravity than what is currently available, but the methods of quantum thermodynamics, combined with the classical Friedman equations for the macroscopic space-time, allow us to describe such an irreversible relaxation in broad strokes. On the question of the size of the initial perturbation that triggers the relaxation, [14] invokes another analogy to a phase transition: the phenomenon of Dicke superradiance in quantum optics [43, 44].

Despite our limited understanding of quantum gravity, our results may have something to say about point (a) in the list given in Sec. I: the problem of the very small entropy of the initial state of the Universe. Our picture is

consistent with taking the initial state of the Universe to be the Bunch-Davies vacuum [41] with $\rho_{\mathrm{dS}} \sim M_{\mathrm{Pl}}^4$ (the "large cosmological constant"). An observer with access only to a sub-space of the full Hilbert space of the Universe may see that vacuum state as having positive entropy. The irreversible relaxation of inflation ($\rho_{\mathrm{dS}} \to 0$) described in [14] could therefore be compatible with a pure initial state. That relaxation may be thought of as a tunneling between the initial Bunch-Davies vacuum and a final Minkowski vacuum. Both states are devoid of particles so that, if the negative energy contribution of gravity is included in the total energy, no global conservation ("superselection") prevents such a tunneling.

According to the astronomical evidence first reported in [10, 11], the Universe does not appear to be relaxing steadily towards empty Minkowski space any more, but has instead recently entered a new dS phase in which matter and radiation coexist with $\rho_{\mathrm{dS}} \sim 10^{-123} M_{\mathrm{Pl}}^4$. Our work, unfortunately, has nothing to say about this "small cosmological constant" problem. It might be due to the presence of a condensate with equation of state $w = -1$, fated to evaporate due to the instability of dS space. Perhaps in a more complete theory of quantum gravity the adiabatic relation between the bath energy density ρ_{dS} to the Hubble parameter h, used in [14], might break down at some time after the end of inflation, obstructing the further relaxation of ρ_{dS}. Note also that in all our calculations the background fields were taken to be massless. This is a good approximation for the early Universe, when h was close to the Planck scale, but the effect of particle masses on the thermodynamics of a dS space at the current, much smaller value of h requires further investigation.

V. DISCUSSION AND OUTLOOK

In this paper we have applied the analytical machinery of quantum thermodynamics, based on the MME for an open system, to the local physics as seen by an observer in dS space whose space-time metric takes the FLRW form of Eq. (1) (the "cosmic rest frame"). Though widely used in quantum optics and some other areas of physics, such analytical techniques have, to our knowledge, not been applied before in the context of dS thermodynamics. This may be partly because they require a non-covariant formulation, which can seem problematic from the point of view of GR. However, because thermodynamic quantities are non-covariant [25] and because cosmology is principally concerned with the physics as it appears to an observer in the cosmic rest frame, we regard this as a useful feature of the MME approach.

We showed that an observer in the cosmic rest frame will see a local system weakly coupled to a background massless quantum field as subject to a black-body radiation with temperature $T_{\mathrm{dS}} = h/2\pi$. Unlike in [4], where this temperature was first computed, we find that other inertial observers do not measure the same T_{dS}, but instead see the radiation as out of equilibrium because the Doppler shifts of the mode frequencies break the KMS condition. This property allows us to interpret T_{dS} as the temperature of a *physical* bath with an energy density obeying the Stefan-Boltzmann law ($\rho_{\mathrm{dS}} \propto T_{\mathrm{dS}}^4$). If this result is extended adiabatically to the case of slowly decreasing h, the back-reaction of ρ_{dS} on the space-time may be taken into account via the Friedmann equations from classical GR. In that case, we find that h relaxes irreversibly towards zero via particle production. This supports previous arguments for the IR-instability of dS space, such as those offered in [15–23], while clearing up some of the obscurity that has surrounded the thermodynamics of dS space. The implications of these results for cosmology are covered in [14].

In [14] we also propose that the primordial perturbations that seed structure formation in the Universe, generally interpreted as resulting form the "freeze-in" of vacuum fluctuations, may be interpreted instead as arising from the thermal fluctuations described by the power spectrum $\mathcal{P}_{\mathrm{th}}(\omega)$ in Eq. (31). This proposal is akin to that of "warm inflation" (see [45, 46] and references therin), except that in our case the temperature of the fluctuations is given directly by the h of inflation and that the thermal fluctuations are obtained from the quantum noise spectra that we introduced in Sec. III C, rather than from a classical Langevin equation. Moreover, our picture does not invoke an inflaton potential $V(\phi)$, or even a coherent inflaton field ϕ. It is clear that such perturbations will be adiabatic, Gaussian, and approximately scale invariant, but detailed calculation of cosmological observables in such a qualitatively new implementation of inflation requires further investigation and the development of a calculational framework not based on a coherent inflaton.

In addition to clarifying the thermodynamics of dS space and inflation, we believe that the MME framework developed in this article can offer a new theoretical tool for understanding the history of the early Universe in terms of out-of-equilibrium, irreversible dynamics. This irreversibility entirely breaks the (approximate) time-reversal symmetry of the underlying microphysics. Cohen and Kaplan have shown that the breaking of the (microphysically exact) CPT invariance by the time-dependent background during inflation allows baryogenesis without CP violation and while baryon-violating interactions are still in equilibrium, circumventing the Sakharov conditions [47]. We believe that the problem of baryogenesis should, therefore, be re-examined in light of the irreversible dynamics of the early Universe.

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Appendix A: Open-system formalism

For the convenience of readers who might not be familiar with the analytical methods for open quantum systems as covered, e.g., in [39], we include in this Appendix a brief summary of salient points of the general derivation of the MME as they are relevant to the present work. A similar but slightly more extensive summary is given in the appendix of [29]. For an interesting review of the history of the development of this formalism, see [48]. As we pointed out at the beginning of Sec. III, the MME has been previously applied to cosmology to describe pure decoherence effects (see, e.g., [38] and references therein), whereas we are interested in using it to describe the thermodynamics of dS space.

The MME describes the non-unitary evolution of the reduced density matrix $\hat{\rho}(t)$ of an open system S weakly coupled to a bath B in stationary state $\hat{\rho}_B$. The system and bath Hamiltonians are denoted by $\hat{H}_0$ and $\hat{H}_B$, respectively. The interaction Hamiltonian is taken to be the product of two Hermitian operators

$$\lambda \hat{H}_{\text{int}} = \lambda \hat{S} \otimes \hat{B}, \tag{A1}$$

with the constant λ giving the strength of the coupling. We may always assume that $\text{Tr}\left(\hat{\rho}_B \hat{B}\right) = 0$. The reduced dynamics of S is expressed in the interaction picture:

$$\hat{\rho}(t) = \Lambda(t,0)\hat{\rho} \equiv \text{Tr}_B\left[\hat{U}_\lambda(t,0)\hat{\rho} \otimes \hat{\rho}_B \hat{U}_\lambda(t,0)^\dagger\right], \tag{A2}$$

for

$$\hat{U}_\lambda(t,0) = \mathbf{T}\exp\left[-i\lambda \int_0^t ds\, \hat{S}(s) \otimes \hat{B}(s)\right], \tag{A3}$$

(where the symbol $\mathbf{T}$ indicates time ordering), with

$$\hat{S}(t) = e^{i\hat{H}t}\hat{S}e^{-i\hat{H}t} \quad \text{and} \quad \hat{B}(t) = e^{i\hat{H}_B t}\hat{B}e^{-i\hat{H}_B t}. \tag{A4}$$

Here, $\hat{S}(t)$ is defined in terms of the *renormalized* Hamiltonian

$$\hat{H} = \hat{H}_0 + \lambda^2 \hat{H}_1^{\text{corr}} + \ldots \tag{A5}$$

The terms proportional to powers of λ in Eq. (A5) are Lamb-shift corrections due to the interaction with the bath, which cancel with the uncompensated term $\hat{H} - \hat{H}_0$ that should, in principle, be present in Eq. (A3).

To extract the leading contribution to the reduced dynamics we apply the cumulant expansion

$$\Lambda(t,0) = \exp\sum_{n=1}^\infty \left[\lambda^n \mathcal{K}^{(n)}(t)\right]. \tag{A6}$$

The first term is $\mathcal{K}^{(1)} = 0$ and the leading Born approximation (corresponding to weak coupling) corresponds to taking $\mathcal{K} = \mathcal{K}^{(2)}$, so that

$$\Lambda(t,0) = \exp\left[\lambda^2 \mathcal{K}(t) + O\left(\lambda^3\right)\right]. \tag{A7}$$

By direct comparison of the cumulant expansion of Eq. (A6) and Dyson expansion for Eq. (A2) we get that

$$\mathcal{K}(t)\hat{\rho} = \int_0^t ds \int_0^t du\, G(s-u)\hat{S}(s)\hat{\rho}\hat{S}^\dagger(u) + \text{(similar terms)}, \tag{A8}$$

where the *bath correlation function* is

$$G(s) \equiv \text{Tr}\left[\hat{\rho}_B \hat{B}(s)\hat{B}\right]. \tag{A9}$$

The "similar terms" in Eq. (A8) are of the form $\hat{\rho}\hat{S}(s)\hat{S}^\dagger(u)$ and $\hat{S}(s)\hat{S}^\dagger(u)\hat{\rho}$.

In the interaction picture, the Markovian approximation, which is valid for sufficiently long times t, is

$$\mathcal{K}(t) \simeq t\mathcal{L}, \tag{A10}$$

where $\mathcal{L}$ is the Gorini-Kossakowski-Lindblad-Sudarshan (GKLS) generator [12, 13]. We decompose $S(t)$ into its Fourier components

$$\hat{S}(t) = \sum_{\{\omega\}} e^{i\omega t} \hat{S}_\omega, \quad \text{with} \quad \hat{S}_{-\omega} = \hat{S}_\omega^\dagger, \tag{A11}$$

where the set $\{\omega\}$ contains the "Bohr frequencies" of the Hamiltonian:

$$\hat{H} = \sum_k \epsilon_k |k\rangle\langle k|, \quad \omega = \epsilon_k - \epsilon_l. \tag{A12}$$

This allows us to write Eq. (A8) in the form

$$\mathcal{K}(t)\rho = \sum_{\omega,\omega'} \hat{S}_\omega \hat{\rho} \hat{S}_{\omega'}^\dagger \int_0^t du \, e^{i(\omega-\omega')u} \int_{-u}^{t-u} d\tau \, G(\tau) e^{i\omega\tau} + (\text{similar terms}). \tag{A13}$$

Applying the approximations

$$\int_0^t du \, e^{i(\omega-\omega')u} \approx t\delta_{\omega\omega'} \quad \text{and} \quad \int_{-u}^{t-u} d\tau \, G(\tau) e^{i\omega\tau} \approx \tilde{G}(\omega) \equiv \int_{-\infty}^\infty d\tau \, G(\tau) e^{i\omega\tau} \geq 0, \tag{A14}$$

which make sense for $t \gg \max\{1/(\omega-\omega')\}$, we obtain that

$$\mathcal{K}(t)\hat{\rho} = t \sum_\omega \tilde{G}(\omega) \hat{S}_\omega \hat{\rho} \hat{S}_\omega^\dagger + (\text{similar terms}) \equiv t\mathcal{L}, \tag{A15}$$

where $\tilde{G}(\omega)$ is called the bath's *spectral density*. Using the commutation of $\mathcal{L}$ with $[H, \cdot]$ one can easily return to the Schrödinger picture and obtain the final MME:

$$\begin{aligned}
\frac{d\hat{\rho}}{dt} &= -i\left[\hat{H}, \hat{\rho}\right] + \mathcal{L}\hat{\rho}, \\
\mathcal{L}\hat{\rho} &\equiv \frac{\lambda^2}{2} \sum_{\{\omega\}} \tilde{G}(\omega) \left(\left[\hat{S}_\omega, \hat{\rho}\hat{S}_\omega^\dagger\right] + \left[\hat{S}_\omega\hat{\rho}, \hat{S}_\omega^\dagger\right]\right).
\end{aligned} \tag{A16}$$

The following points are important to bear in mind:

(i) The absence of off-diagonal terms in Eq. (A16), compared to Eq. (A13), is the crucial property, which can be interpreted as a coarse-graining in time of rapidly oscillating terms (the "secular approximation"). It implies the commutation of $\mathcal{L}$ with the Hamiltonian part $[\hat{H}, \cdot]$.

(ii) The positivity $\tilde{G}(\omega) \geq 0$ follows from Bochner's theorem and is a necessary condition for *complete positivity* of the MME, which is a fundamental property of quantum dynamics that prevents the occurrence of negative probabilities. When applying this formalism to a particular open system, this positivity of the bath's spectral density can provide a useful sanity check: see, e.g., Eq. (53) in the main text.

(iii) For more complicated interaction Hamiltonians of the form $\hat{H}_{\text{int}} = \sum_\alpha \hat{S}_\alpha \otimes \hat{B}_\alpha$ we replace $\tilde{G}(\omega)$ by the positive-definite relaxation matrix $\tilde{G}_{\alpha\beta}(\omega)$, which (because of symmetry) is usually diagonal in an appropriate parametrization.

(iv) Point (i) implies that the diagonal elements of the density matrix (in the energy representation) evolve independently of the off-diagonal ones. They satisfy the Pauli Master Equation, with transition rates equal to those calculated from Fermi's golden rule [49].

If the reservoir is a quantum system in a thermal equilibrium state, the bath's spectral density must obey the KMS condition

$$e^{-\beta\omega} = \frac{\tilde{G}(-\omega)}{\tilde{G}(\omega)}, \tag{A17}$$

where β is the bath's inverse temperature ($\beta = 1/T$). As a consequence of Eq. (A17), the Gibbs state

$$\hat{\rho}_\beta = Z^{-1} e^{-\beta\hat{H}}, \tag{A18}$$

is a stationary solution of Eq. (A16). Under mild conditions (e.g., that the only system operators commuting with $\hat{H}$ and $\hat{S}$ are scalars) the Gibbs state is a unique stationary state and any initial state relaxes towards equilibrium ("zeroth law of thermodynamics"). One can also show that the second law of thermodynamics is fulfilled in the sense that entropy production is positive.

Note that if an observer sees the bath moving, the Doppler shifts of the ω's in Eq. (A17) will break the KMS condition, so that the bath will not fulfill the zeroth law of thermodynamics with respect to that observer. Sewell showed in [25] that temperature cannot, therefore, be defined covariantly in quantum physics. Some of the physical consequences of such Doppler shifts have been studied in [29, 30].