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Modave lectures on quantum cosmology: wavefunction of the universe, no-boundary proposal and gravitational path integrals

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These notes aim to provide a pedagogical introduction to the subject of quantum cosmology: the study of the very early universe including quantum effects. We assume previous knowledge of general relativity and quantum field theory. Basic knowledge in cosmology is ideal but for those unfamiliar with this topic we briefly review the key notions in the introduction (good lecture notes and books more comprehensive on this topic are for instance: Baumann 2009 [1] and Mukhanov 2005 [2]).

We start by reviewing the early attempt to canonically quantize gravity. We explain how this led to the concept of a wavefunction of the universe together with the Wheeler-de Witt equation governing it. Then we turn to the no-boundary [3, 4] and tunneling [5, 6] proposals and review the many successive endeavors to make these proposals concrete in simplified models. We finally study in detail the Euclidean and Lorentzian gravitational path integrals, including some tools used in this context such as the BRST procedure and the Picard-Lefschetz theory of complex analysis.

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PoS(Modave2024)003

1. Introduction

1.1 What is quantum cosmology?

The basic idea behind quantum cosmology is very simple: quantum mechanic seems so far to be universal, therefore it should apply to the universe as a whole. In the 20th century, general relativity (GR) enabled a jump in our ability to model the universe through the spatially homogeneous and isotropic FLRW metric:

$$\mathrm{d}s^2 = -N^2\mathrm{d}t^2 + a(t)^2\mathrm{d}\vec{x}^2\,, \tag{1}$$

leading to the hot big bang model. Given the crude simplicity of the FLRW metric, which describes the geometry of our universe using only one degree of freedom, the scale factor $a(t)$, it seems a miracle that it fits observational data such as the cosmic microwave background (CMB) temperature map so well, see Figure 1. Our early universe seems strikingly homogeneous and isotropic.

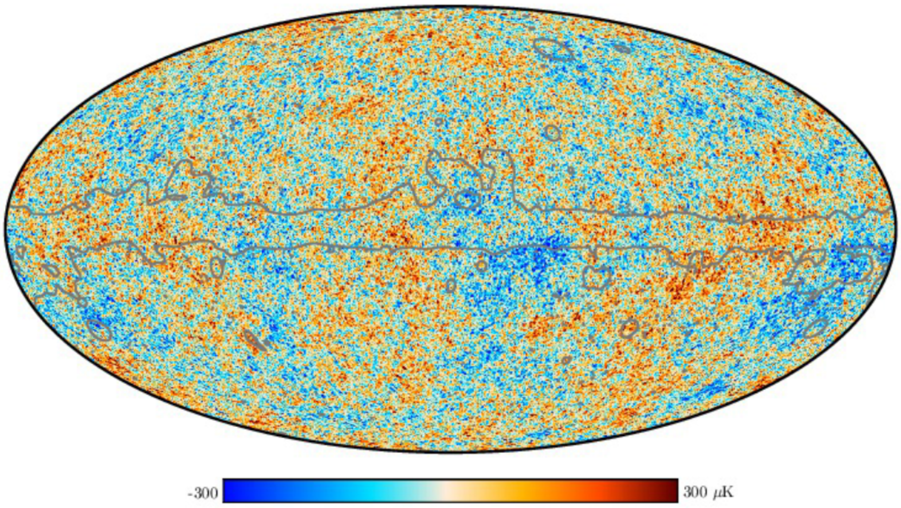

Figure 1: All-sky map of the fluctuations of temperature observed in the cosmic microwave background by the Planck's satellite. The average temperature is $T_{\rm CMB} = 2.72548 \pm 0.00057K$, and the fluctuations range from $-300\,\mu$K to $+300\,\mu$K around that value. This represents a ratio of variation of about $\delta T/T \sim 10^{-4}$ over the entire observable universe. Figure taken from [7].

Moreover, since this FLRW model predicts that our universe is shrinking when going backward in time, we can naively expect that the universe once had a quantum scale. Of course we can legitimately cast doubts on the validity of the classical GR theory at that point, especially since quantization of the said GR theory fails (i.e., when loop corrections are taken into account, they generate effective higher order curvature terms) [8–10]: GR cannot be quantized using the ordinary perturbative approach. Despite decades of efforts, we are still far from understanding what quantum gravity is.

Quantum cosmology suggests a middle ground: instead of trying to quantize gravity in its full glory, we focus our attention to the specific case of the very early universe and study quantum effects arising in this context. In these notes we will study the path integral quantization and the canonical quantization methods. There, one uses semi-classical approaches such as the saddle-point approximation of path integrals in order to carry concrete calculations and capture certain

PoS(Modave2024)003

quantum effects, for instance the competition of different branches. In principle these two methods can describe all the 10 degrees of freedom of GR, but in practice we often restrict to quantizing only a few fields in a first toy-model approximation, in the hope that this can already capture some important features while keeping calculations tractable. In that case we say that we reduce to minisuperspace[1]. This (huge) truncation of the number of degrees of freedom cannot be justified from the dynamic of the system. In that sense it really is only a toy model, even though we hope to learn about some features of the early universe (or at least get a better understanding of the mathematical tools we are using to describe this system), given how the classical picture fits with FLRW.

Ultimately the golden aim of the study of the early universe is to match theory with observations (such as the Planck data [7]), and recent advances in quantum cosmology are attempting to bridge this gap with the approaches of top-down quantum cosmology [13] and more recently using the Kontsevich-Segal criterion for complex metric [14–16].

Some further caveat: quantum gravity is more than quantum field theory on curved spacetime, yet even the latter isn't fully understood (especially for instance on spacetimes like de Sitter). Our approach is necessarily deficient by its very search for simplicity, yet it often offers the only computable examples at hand. Going beyond the approximations made here, e.g., beyond minisuperspace or beyond the simple action of GR, are necessary steps toward a more comprehensive theory of the early universe.

Conclusion: we do what we can so far with the tools we already have, even though we fully know it's not complete, and we try to see if this partial theory already brings some answers/ explains part of the observational data. Then we try to extend it beyond the most simplistic assumptions and see what still holds.

The plan of these notes is as follow: I will start by quickly reviewing the standard model of cosmology, namely the FLRW model of the universe as well as its most common extension, the theory of inflation. We will then argue for the necessity of some sort of theory of initial conditions. In section 2 we will dive into the first canonical quantization attempt of gravity and be led for the first time to the notion of *wavefunction of the universe*. In section 3 we will introduce the no-boundary and tunneling proposals as contenders for a theory of initial conditions. We will follow the subsequent development of these proposals in sections 3 and 4, reviewing both the Euclidean and Lorentzian path integral approaches, hence providing an overview of the different viewpoints.

Even within the small subfield of quantum cosmology, there are many topics that these notes must bypass. A non-exhaustive list with a few references to go further includes:

- the EAdS/dS holographic point of view of quantum cosmology [17];
- 2D quantum cosmology [11];
- recent developments on the tunneling proposal [18, 19];
- resurgence theory and discussion of the Stokes phenomenon [20, 21];

etc.

[1]Other simplified approaches to quantum cosmology include the reduction of dimensions [11] or the limit of asymptotic future infinity [12].

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1.2 FLRW cosmology & inflation

Very soon after the advent of the classical theory of general relativity came its first application to the description of our whole universe. Friedmann[2] found in 1924 that the Einstein field equations possessed a solution for a spatially homogeneous and isotropic universe, yet expanding in time. The assumption of spatial homogeneity and isotropy is known as the cosmological principle, and it was since then found to be valid in our universe to a very good approximation on large scales, most spectacularly by the CMB, whose latest measurement by the Planck satellite [22] is reproduced in Figure 1. Friedmann's spatially homogeneous and isotropic solution is given by the **FLRW metric**:

$$\mathrm{d}s^2 = -N(t)^2\mathrm{d}t^2 + a(t)^2\left(\frac{\mathrm{d}r^2}{1-kr^2} + r^2\mathrm{d}\Omega_2^2\right) . \tag{2}$$

Locally, this is the unique spatially homogeneous and isotropic metric in four dimensions, but globally there might be different spacetimes associated with different topologies. The FLRW metric features a drastic reduction of the number of degrees of freedom: instead of a metric whose evolution varies at every single point in spacetime (i.e., infinitely many functions of time), our system is described by only two functions of time $a(t)$ and $N(t)$. k is the spatial curvature, that can take values 0, 1 or -1 (resp. spatially flat, close or open). Plugging this metric into Einstein's field equations,

$$R_{\mu\nu} - \frac{1}{2}g_{\mu\nu}R - \Lambda g_{\mu\nu} = 8\pi G\, T_{\mu\nu}\, , \tag{3}$$

and assuming a stress-energy tensor accounting for a perfect fluid matter with equation of state (EoS) $p(t) = w\rho(t)$:

$$T^{\mu\nu} = p(t)g^{\mu\nu} + (\rho(t) + p(t))\, u^\mu u^\nu\, , \tag{4}$$

where $\rho(t)$ is the energy density, $p(t)$ the pressure and u^μ the four-velocity, we obtain the Friedmann constraint and equations of motion of an homogeneous and isotropic universe:

$$\begin{cases} \dfrac{3H^2}{N^2} + \dfrac{3k}{a^2} = \Lambda + 8\pi G\rho \quad \text{(Friedmann constraint)}\, , \\ \dfrac{2\dot{H}}{N^2} + \dfrac{3H^2}{N^2} + \dfrac{k}{a^2} = \Lambda - 8\pi G p \quad \text{(acceleration equation)}\, , \\ \dot{\rho} + 3H(\rho + p) = 0 \quad \text{(continuity equation)}\, , \end{cases} \tag{5}$$

with $H = \dot{a}/a$ the Hubble rate[3].

The above cosmological equations yield different regimes of evolution for the scale factor depending on the matter content dominating the universe. There are three main types of matter content that must be considered. First **radiation** (aka photons), characterized by an EoS $p_\gamma = \rho_\gamma/3$, implying that $\rho_\gamma(t) = \rho_\gamma(t_0)\, a(t_0)^4/a(t)^4$. Second comes **non-relativistic matter** (ordinary and cold dark matter) with EoS $p_\mathrm{M} = 0$, $\rho_\mathrm{M} \neq 0$, hence $\rho_\mathrm{M} = \rho_\mathrm{M}(t_0)\, a(t_0)^3/a(t)^3$. Finally the

[2] This solution was also found by Lemaître in 1927, and then by Robertson and Walker in 1935, hence the name Friedmann-Lemaître-Robertson-Walker (FLRW).

[3] The measured quantity nowadays is of about $H(t_0) \equiv H_0 \simeq 70\,\mathrm{km\,s^{-1}Mpc^{-1}}$. The Planck's measurement gives $H_0 = 66.88 \pm 0.92\,\mathrm{km\,s^{-1}Mpc^{-1}}$ [22], while the local measurement based on the distance-redshift velocity relation for Cepheids and type Ia supernovae yields $H_0 = 73.00 \pm 1.75\,\mathrm{km\,s^{-1}Mpc^{-1}}$ [23]. The tension between these values is still unexplained and has provoked a reconsideration in recent years of the standard model of cosmology.

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third type of matter content is **vacuum energy** (aka the cosmological constant). Indeed in the cosmological equations (5), the cosmological constant terms can be understood as an additional type of matter with energy density $\rho_\Lambda \equiv \Lambda/(8\pi G)$ and pressure $p_\Lambda \equiv -\Lambda/(8\pi G)$. This energy density is time-independent.

Accounting for these three types of matter content, the Friedmann equation becomes:

$$H^2 + \frac{k}{a^2} = \frac{8\pi G}{3} \left(\rho_\gamma + \rho_{\mathrm{M}} + \rho_\Lambda\right), \tag{6}$$

$$\Rightarrow \text{ at } t = t_0: \quad 1 + \frac{k}{a(t_0)^2 H_0^2} = \frac{8\pi G}{3H_0^2} \left(\rho_\gamma(t_0) + \rho_{\mathrm{M}}(t_0) + \rho_\Lambda\right). \tag{7}$$

The quantity $\rho_c \equiv 3H_0^2/(8\pi G)$ is called the critical density[4]. The equation (7) provides the abundances ratio of each matter content at present time $t = t_0$: $\Omega_\gamma \equiv \rho_\gamma(t_0)/\rho_c$, $\Omega_{\mathrm{M}} \equiv \rho_{\mathrm{M}}(t_0)/\rho_c$ and $\Omega_\Lambda \equiv \rho_\Lambda/\rho_c$ are respectively the radiation, matter and cosmological constant abundances. By similarly defining the spatial curvature abundance as $\Omega_k \equiv -k/(a(t_0)^2 H_0^2)$, we can rewrite equation (7) as $1 = \Omega_\gamma + \Omega_{\mathrm{M}} + \Omega_\Lambda + \Omega_k$. Using the time dependencies of the energy density for the different matter types, we can express the Friedmann equation in term of the energy density abundances:

$$H(t)^2 = H_0^2 \left[\Omega_\Lambda + \Omega_{\mathrm{M}} \frac{a(t_0)^3}{a(t)^3} + \Omega_\gamma \frac{a(t_0)^4}{a(t)^4} + \Omega_k \frac{a(t_0)^2}{a(t)^2}\right]. \tag{8}$$

This equation yields three different regimes of evolution depending on which term dominates the energy content in time. From experimental data, we measure that $\Omega_\Lambda = 0.6847 \pm 0.0073$, $\Omega_{\mathrm{M}} = 0.315 \pm 0.007$, $\Omega_k = 0.0007 \pm 0.0019$ [5] [22] and $\Omega_\gamma = 5.38 \cdot 10^{-5}$ [24]. Therefore at present time, the term ρ_Λ dominates the equation (8) and leads to a cosmological constant dominated era with an approximate exponential evolution for the scale factor (approximate de Sitter spacetime): $a(t) \sim e^{H \cdot t}$, and $H = \sqrt{\Lambda/3}$.

Going backward in time, the scale factor a shrinks, and the matter and radiation terms $\Omega_{\mathrm{M}}/a(t)^3$ and $\Omega_\gamma/a(t)^4$ grow, until they turn by turn dominate the equation (8).

First the matter content dominates: before the time t_1 where $\rho_{\mathrm{M}}(t_1) = \rho_\Lambda(t_1)$, the scale factor approximately evolves as $a(t) \sim t^{2/3}$ and $H(t) = 2/(3t)$. Finally, the radiation content dominates before the time t_2 where $\rho_\gamma(t_2) = \rho_{\mathrm{M}}(t_2)$ and the scale factor evolves as: $a(t) \sim t^{1/2}$ and $H(t) = 1/(2t)$.

These three regimes of evolution are depicted in Figure 2. In principle there could be a spatial curvature dominated era in-between the matter and cosmological constant ones, but the smallness of Ω_k prevents that term from dominating before the matter term starts prevailing.

The radiation and matter dominated eras consist in power law evolutions for the scale factor $a(t) \sim t^\alpha$. This implies that at some point in time, $a \to 0$ and $\rho \to +\infty$. This corresponds to the so-called big bang or cosmological singularity. The above analysis does not include quantum effects, which cannot be neglected anymore when $\rho \to +\infty$. The model breaks down when $\rho \sim M_{\mathrm{Pl}}^4$, corresponding to a time scale of $t \sim 1/M_{\mathrm{Pl}} \sim 10^{-43}$ s. The evolution described above is theoretically

[4] It is called critical density because depending on whether its ratio with the present total energy density $(\rho_\gamma^0 + \rho_{\mathrm{M}}^0 + \rho_\Lambda)$ is smaller than, equal to or larger than 1, the spatial curvature of our present universe will be open, flat or closed.

[5] This explains why our late-universe model is named the ΛCDM model, since the two largest components of the energy content nowadays are the vacuum energy and cold dark matter.

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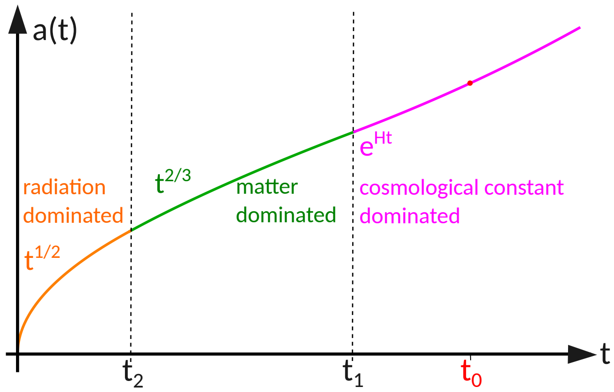

Figure 2: Approximated regimes of evolution of the scale factor in time following the hot big bang model. Present time t_0 is represented by a red dot, and is estimated to be 13.8 billion years. The transition from radiation to matter dominated epoch takes place about 50 000 years after the big bang. The transition from matter dominated to cosmological constant dominated phase takes place about 10 billion years after the big bang, very recently compared to the total age of the universe.

valid up to that point, which enables to get to states with very large densities, larger than the density inside atomic nuclei. This statement forms the basis of the hot big bang model, first proposed by Gamow in 1948, which assumes that the early universe was in a thermal equilibrium at a certain temperature and density, reaching hotter and denser states while going back in time. This model led to the prediction of the CMB (confirmed experimentally by Penzias and Wilson in 1965) and of the primordial abundance of light elements (big bang nucleosynthesis), also confirmed by the composition of early stars. Despite its simplicity, this model thus approximates very well the early universe.

However, in addition to the fact that GR cannot be trusted above the Planck scale, the big bang model requires extremely fine-tuned initial conditions. This is exemplified by the so-called horizon and flatness puzzles, and led to the addition of inflation[6] to the standard model of cosmology.

The **horizon puzzle** results from the fact that in a power-law expanding universe $a(t) \sim t^\alpha$, the size of causally connected regions that we observe in the CMB should be of the order of a few degrees[7], in stark contrast with the homogeneity we observe in the full sky.

[6] Alternatives to inflation also resolving the fine-tuning issues and still in agreement with current observations include bouncing models [25] as well as loitering phases (as in string gas cosmology [26]). All these theoretical models, including inflation, are expected to be confirmed or ruled out by the (non-)observation of tensor perturbations in the CMB.

[7] Explicitly, the finite bound on the speed of propagation c implies that any two events whose spatial separation ℓ is larger than $c \cdot \Delta t$, where Δt is their time separation, cannot be causally connected. In an expanding universe, the size of the causal horizon $\ell(t)$ is deformed by the Hubble rate of expansion $H(t) = \dot{a}(t)/a(t)$:

$$\frac{\mathrm{d}\ell}{\mathrm{d}t} = c + \frac{\dot{a}(t)}{a(t)} \cdot \ell \;\Leftrightarrow\; \ell(t) = c \cdot a(t) \int_{t_\mathrm{ini}}^{t} \frac{\mathrm{d}t'}{a(t')} = c \cdot t^\alpha \int_{t_\mathrm{ini}}^{t} \frac{\mathrm{d}t'}{t'^{\,\alpha}} \quad \text{for } a(t) \propto t^\alpha \,.$$

When the initial time $t_\mathrm{ini} \to 0$, the above integral converges for $\alpha < 1$ and yields $\ell(t)|_{t_\mathrm{ini}=0} = \frac{t}{1-\alpha}$. Therefore, at the time of recombination of electrons, which approximately corresponds to the CMB time, the size of the causal horizon is $\ell_\mathrm{CMB} \sim 3\, t_\mathrm{CMB}$, because we are in the matter dominated epoch for which $\alpha = 2/3$. After the expansion of the universe, we observe this causal region at present time as a region of size: $\ell(t_0) \equiv \ell_\mathrm{CMB} \cdot \frac{a(t_0)}{a(t_\mathrm{CMB})} \sim 3\, t_\mathrm{CMB}^{1/3} t_0^{2/3}$. The angular region we observe in the sky now and that should have been causally connected at the time of the CMB has a size of $\theta \simeq \ell(t_0)/(3t_0) = (t_\mathrm{CMB}/t_0)^{1/3} = 2^\circ$, since $t_\mathrm{CMB} \sim 5 \cdot 10^5$ years and $t_0 \sim 15 \cdot 10^9$ years.

PoS(Modave2024)003

The **flatness puzzle** is more controversial and concerns the smallness of the spatial curvature measured today. From the Friedmann equation (8), we expect the curvature term $\Omega_k a(t_0)^2/a(t)^2$ to dominate as the scale factor grows, but instead we observe it to be very small at present, meaning it must have started from an unnaturally small value in the past (that is, assuming it is non-zero)[8].

These two puzzles are both a consequence of the scale factor evolving as a power-law down to the singularity at $t \to 0$. However the hot big bang model has been experimentally confirmed only down to about $t \sim 1$s by the big bang nucleosynthesis. One can therefore imagine another phase of evolution taking place before that experimentally checked time which would resolve these puzzles. This is precisely what inflation does (but this is also how alternatives to inflation such as bounces or loitering phases work).

Inflation assumes a phase of accelerated expansion taking place before the radiation dominated era. Such an evolution can be generated by a perfect fluid with EoS $p = w\rho$ and $-1 < w < -1/3$. It can solve the horizon and flatness puzzles in a very short time period, around 10^{-36} to 10^{-34} seconds in some simple models [2]. This would stay consistent with even very conservative hot big bang evolutions going back further than the electroweak scale (10^{-12}s). A vanilla implementation of this scenario, relying on quantum field theory on curved backgrounds, is the scalar field inflation. The simplest case, although ruled out by observation, is a massive scalar field minimally coupled to gravity[9]:

$$S = \int \mathrm{d}^4x\sqrt{-g}\left(\frac{R}{16\pi G} - \frac{1}{2}g^{\mu\nu}\partial_\mu\phi\partial_\nu\phi - \frac{m_\phi^2\phi^2}{2}\right). \tag{9}$$

In most models of inflation, the inflaton – here the massive scalar – is taken to be a homogeneous and isotropic field from the onset. Therefore, contrary to a naive understanding, **inflation does not explain why our early universe was homogeneous and isotropic**. Instead, it resolves the fine-tuning and causality paradoxes exposed earlier, but it still requires very special initial conditions to start with. This is precisely the missing piece that quantum cosmology tries to address: providing a theory of initial conditions able to predict the homogeneity and isotropy we observe.

For completeness we quickly review here the mechanism of **slow-roll inflation**. The equations of motion associated with the action (9) assuming an FLRW metric (again we assume homogeneity and isotropy from the start) are

$$H^2 + \frac{k}{a^2} = \frac{8\pi G}{3}\left(\frac{\dot{\phi}^2}{2} + \frac{m_\phi^2\phi^2}{2}\right)\ ; \quad \ddot{\phi} + 3H\dot{\phi} + m_\phi^2\phi = 0\,. \tag{10}$$

The $3H\dot{\phi}$ in the scalar field equation is a friction term due to the expansion of the universe. If $H = 0$, the scalar field oscillates indefinitely in the potential, but when H becomes larger and larger, this

[8]More precisely, the Friedmann equation (6) provides a measuring tool of the spatial curvature of the universe: $\frac{k}{a^2H^2} = \Omega - 1$, where $\Omega \equiv 8\pi G\,\frac{\rho_\gamma + \rho_\mathrm{M} + \rho_\Lambda}{3H^2}$. For the spatially flat case $k = 0$, we find that the quantity $\Omega = 1$ is time-independent. Otherwise, Ω is time dependent and in particular, for a scale factor $a \sim t^\alpha$ with $\alpha < 1$, we find that $H \sim 1/t$, so that $\Omega - 1 \sim k\cdot t^{2-2\alpha}$. At present time we measure $\Omega - 1 \sim 10^{-2}$, so evolving this quantity backward in time until for example the big bang nucleosynthesis time where $t \sim 1$s, we find that the spatial curvature was $\Omega - 1 \sim 10^{-15}$. The other way around, it looks as if the initial value for the Hubble rate had been hugely fine-tuned so that the present universe was nearly spatially flat.

[9]More realistic models favored by current observations include for example the Higgs inflation [27] or the Starobinsky R^2 inflation [28].

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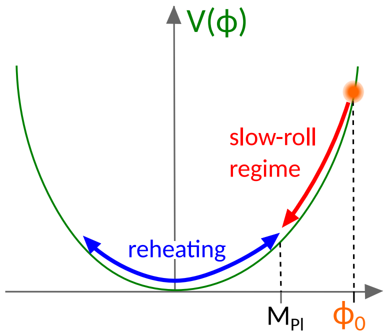

Figure 3: Sketch of the inflationary slow-roll mechanism. The inflaton field (in orange) starts from a value $\phi_0 > M_{\rm Pl}$ and rolls down the potential in the slow-roll regime, producing an accelerated expansion. When it exits this regime, it reaches the oscillatory reheating phase.

oscillation gets more and more damped. We focus on a specific regime for which the oscillations are overdamped, characterized by: $\ddot{\phi} \ll 3H\dot{\phi}$ and $\dot{\phi}^2 \ll m_\phi^2\phi^2$, the slow-roll regime. In this regime the equations (10) become

$$3H\dot{\phi} + m_\phi^2\phi \simeq 0\,, \quad H^2 \simeq \frac{8\pi G}{3}\frac{m_\phi^2\phi^2}{2}\,. \tag{11}$$

The solution to these equations for the scalar field is $\phi(t) \simeq \phi_i - m_\phi(t-t_i)/\sqrt{12\pi G}$. From the slow-roll condition $|\dot{\phi}| \ll |m_\phi \phi|$, we deduce that this solution is valid only for $\phi(t) \gg \frac{1}{\sqrt{12\pi G}} \equiv \sqrt{\frac{2}{3}}M_{\rm Pl}$. Assuming that the initial scalar field value ϕ_i satisfies this condition[10], we find the solution for the scale factor as $a(t) \simeq a_i \exp\left(\frac{m_\phi}{\sqrt{6}\,M_{\rm Pl}}\left(\phi_i(t-t_i) - \frac{M_{\rm Pl} m_\phi (t-t_i)^2}{\sqrt{6}}\right)\right)$.

We obtain the sought-after accelerated expansion, valid as long as $t - t_i \lesssim \sqrt{\frac{3}{2}}\,\phi_i/(M_{\rm Pl}\,m_\phi)$. When we reach $\phi_{\rm critical} = \sqrt{\frac{2}{3}}M_{\rm Pl}$, i.e., at $t_{\rm critical} - t_i = \sqrt{\frac{3}{2}}\,\phi_i/(M_{\rm Pl}\,m_\phi)$, the slow roll approximation breaks down and the accelerated expansion stops. The $\ddot{\phi}$ term in (10) cannot be neglected anymore, and we obtain an oscillatory behavior for the scalar field where reheating [29] takes place, giving rise in principle to all the standard model elementary particles. From then on the universe starts following the hot big bang evolution described earlier (see Figure 3 for an illustration). The total amount of expansion produced by the inflationary phase is of about $a_{\rm critical}/a_i \simeq \exp\left(\frac{\phi_i^2}{4M_{\rm Pl}^2}\right)$: the exponent $\phi_i^2/(4M_{\rm Pl}^2)$ is called the e-fold number and must be of order 60 for the flatness and horizon problem to be solved [30]. This means that for this model of inflation, we find that inflation must last for a period of time $\Delta t \equiv t_{\rm critical} - t_i = \sqrt{\frac{3}{2}}\frac{\phi_i}{M_{\rm Pl}\,m_\phi} \simeq 10^{-12}\,{\rm GeV}^{-1} \simeq 10^{-36}$ s for $m_\phi \simeq 10^{13}$ GeV, which is the typical mass of the inflaton needed to explain density fluctuations in the CMB [2].

[10]This is justified because the scalar field value is not an observable, but its energy density, $\dot{\phi}^2 + m_\phi^2\phi^2$, is. In the classical regime, this energy density must be much smaller than the Planck density energy $\rho \sim M_{\rm Pl}^4$, while the mass of the scalar field must be much smaller than the Planck mass: $m_\phi^2 \cdot \phi^2 \ll M_{\rm Pl}^4$ and $m_\phi \ll M_{\rm Pl}$. Given the huge ratio between the Planck mass and the mass of standard particles, it is reasonable to assume that $\phi_i \gg M_{\rm Pl}$.

PoS(Modave2024)003

2. Canonical quantization and the wavefunction of the universe

Now that we have reviewed the standard take on cosmology, we can begin to explore the very early phases of the universe, where quantum mechanics becomes relevant.Even though GR is non-renormalizable and can thus not be quantized directly, we will start by introducing the method of canonical quantization of gravity, because this will lead us to key notions in quantum cosmology such as the Wheeler-de Witt equation and the wavefunction of the universe. In the next section we will then be in position to introduce the path integral quantization and the no-boundary proposal as a theory of initial conditions for the early universe.

2.1 Hamiltonian formulation of gravity

Canonical quantization is based on the Hamiltonian formulation of gravity, where the metric $\mathrm{d}s^2 = g_{\mu\nu}\mathrm{d}x^\mu \mathrm{d}x^\nu$ is rewritten in the Arnowitt-Deser-Misner [31] form describing the foliation of spacetime in equal-time hypersurfaces:

$$\mathrm{d}s^2 = -N^2\mathrm{d}t^2 + \gamma_{ij}(\mathrm{d}x^i + N^i\mathrm{d}t)(\mathrm{d}x^j + N^j\mathrm{d}t)\,. \tag{12}$$

N is the lapse function, N^i are the shift functions and γ_{ij} is the three-metric on the hypersurface. Up to now this description is fully equivalent to the original GR one, but it enables to perform a Legendre transformation into the Hamiltonian action formulation. To do so, the first step is to use the Gauss-Codacci relation expressing the four-dimensional Ricci scalar R in terms of the three-dimensional one constructed from γ_{ij}, ${}^{(3)}R$, and the extrinsic curvature $K_{ij} \equiv \frac{1}{2N}\left(-\partial_t\gamma_{ij} + 2D_{(i}N_{j)}\right)$:

$$R = K_{ij}K^{ij} - K^2 + {}^{(3)}R\,. \tag{13}$$

Then the Hamiltonian action formulation can be written as:

$$S = \int \mathrm{d}^4x\sqrt{-g}\,(R - 2\Lambda) + S_{\mathrm{matter}} = \int \mathrm{d}t\,\mathrm{d}^3x\,\mathcal{L} = \int \mathrm{d}t\,\mathrm{d}^3x\left[\Pi^{ij}\partial_t\gamma_{ij} - N\mathcal{H} - N^i\mathcal{H}_i\right], \tag{14}$$

where $\Pi^{ij} \equiv \dfrac{\delta\mathcal{L}}{\delta\gamma_{ij}} = -\dfrac{\sqrt{\gamma}}{2}\left(K^{ij} - \gamma^{ij}K\right)$ is the conjugate momentum of the spatial metric γ_{ij} and $\mathcal{H}$, $\mathcal{H}_i$ are the Hamiltonian and spatial diffeomorphism constraints, that appear in the action with their associated Lagrange multipliers N and N^i. Those constraints explicitly read:

$$\begin{cases}\mathcal{H} = G_{ijkl}\Pi^{ij}\Pi^{kl} - \sqrt{\gamma}\left({}^{(3)}R - 2\Lambda\right) + \mathcal{H}_{\mathrm{matter}}\,;\\ \mathcal{H}_i = -2\pi\, D_j\Pi_i{}^j + \mathcal{H}^i_{\mathrm{matter}}\,,\end{cases} \tag{15}$$

with $G_{ijkl} = \dfrac{1}{2\sqrt{\gamma}}\left(\gamma_{ik}\gamma_{jl} + \gamma_{il}\gamma_{jk} - \gamma_{ij}\gamma_{kl}\right)$, the de Witt supermetric[11]. The constraints (15) give rise to the general constraint equations of canonical gravity: $\mathcal{H} = 0$ and $\mathcal{H}_i = 0$. The three latter are linear in the momenta and generate diffeomorphisms within the three-surfaces, similarly to the case of ordinary gauge symmetries. The first Hamiltonian constraint, instead, is quadratic in the

[11] A note on etymology: G_{ijkl} is called the de Witt supermetric because it acts on the so-called "superspace" constiting of the variables γ_{ij} and their momenta Π^{ij}. Hence the name "minisuperspace" when we restrict to a finite number of degrees of freedom, $\gamma_{ij} = a(t)^2\delta_{ij}$.

PoS(Modave2024)003

momenta. Beyond expressing the invariance under time reparametrizations, it also generates the dynamic of the system. By canonically quantizing this theory (i.e., by transforming $\pi^{ij} \to -i\hbar\frac{\partial}{\partial\gamma_{ij}}$), these constraints transform into conditions on the quantum state of the whole universe:

$$\mathcal{H}\Psi = 0 \text{ and } \mathcal{H}_i\Psi = 0\,. \tag{16}$$

The dynamical equation following from the first condition is called the Wheeler-de Witt (WdW) equation and can be thought of as an equivalent of the Schrödinger equation, to the crucial difference that this equation is of second and not first order in time derivatives:

$$\left[-\hbar^2 G_{ijkl}\frac{\partial}{\partial\gamma_{ij}}\frac{\partial}{\partial\gamma_{kl}} - \sqrt{\gamma}\left({}^{(3)}R - 2\Lambda\right) + \mathcal{H}_{\text{matter}}\right]\Psi = 0\,. \tag{17}$$

In other words, time here is a coordinate and not a parameter. This has profound implications for the unitarity of the theory and thus raises ambiguities in the meaning, definition and interpretation of the usual quantum mechanical objects such as the probability distribution, the inner product or the measure. In addition to that, similarly to the Einstein equations in GR, it is technically impossible to solve the WdW equation (17) at every point of spacetime for generic metrics. Instead one has to resort to some (highly) simplified ansatz, namely minisuperspace in the context of this lecture.

2.2 Wheeler-de Witt equation in minisuperspace

The simplest minisuperspace is a homogeneous and isotropic spacetime $\mathrm{d}s^2 = -N^2\mathrm{d}t^2 + a(t)^2\mathrm{d}\Omega_3^2$ with a positive cosmological constant Λ. We also add a minimally coupled massive scalar field for illustration purpose, so that our superspace will be two-dimensional. The action then reads (with $\kappa = 1$)[12]:

$$\begin{aligned}
S_{\text{tot}} &= \int \mathrm{d}^4x\sqrt{-g}\left[\frac{R}{2\kappa} - \Lambda + \frac{1}{2}\partial_\mu\phi\partial^\mu\phi - \frac{m^2\phi^2}{2}\right] + \frac{1}{\kappa}\int \mathrm{d}^3y\sqrt{h}\,K, && (18)\\
&= 2\pi^2\int \mathrm{d}t\,N\left[-\frac{3a\dot{a}^2}{N^2} + 3a - a^3\Lambda + \frac{a^3\dot{\phi}^2}{2N^2} - \frac{a^3m^2\phi^2}{2}\right], && (19)\\
&\equiv \int \mathrm{d}t\,N\left(\frac{G_{AB}\dot{q}^A\dot{q}^B}{2N^2} - U(q^A)\right) = \int \mathrm{d}t\,L(q,\dot{q})\,. && (20)
\end{aligned}$$

The associated de Witt supermetric is $G_{AB} = \begin{pmatrix} -12\pi^2 a & 0 \\ 0 & 2\pi^2a^3\end{pmatrix}$, and the potential reads $U(a,\phi) = 2\pi^2\left(-3a + a^3\Lambda + \frac{a^3m^2\phi^2}{2}\right)$. We can Legendre transform to the Hamiltonian formulation by calculating the conjugated momenta:

$$p_N \equiv \frac{\partial L}{\partial\dot{N}} = 0\,;\quad p_a \equiv \frac{\partial L}{\partial\dot{a}} = -\frac{12\pi^2a\dot{a}}{N}\,;\quad p_\phi \equiv \frac{\partial L}{\partial\dot{\phi}} = \frac{2\pi^2a^3\dot{\phi}}{N}\,. \tag{21}$$

[12]The last term in (18) is the Gibbons-Hawking-York (GHY) term, constructed using the extrinsic curvature of the hypersurface with induced metric h_{ij}: $K = h_{ij}K^{ij}$. It must be added to any surface boundary to enable the boundary value problem to be well defined with Dirichlet boundary conditions. There will be some subtleties for the no-boundary boundary conditions that we will deal with later, but for now we can safely ignore boundary terms.

PoS(Modave2024)003

so that the Hamiltonian reads

$$
\begin{aligned}
H(p_A, q^A) = p_N \dot{N} + p_a \dot{a} + p_\phi \dot{\phi} - L &= \frac{N}{2}\left(-\frac{p_a^2}{12\pi^2 a} + \frac{p_\phi^2}{2\pi^2 a^3} + 2\pi^2\left[-6a + 2\Lambda a^3 + m^2 a^3 \phi^2\right]\right), \\
&\equiv N\left(\frac{G^{AB} p_A p_B}{2} + U(q^A)\right) \equiv N\mathcal{H}. \qquad (22)
\end{aligned}
$$

The lapse does not have a momentum because it is a non dynamical variable that can be viewed as a Lagrange multiplier imposing the Hamiltonian constraint (see (14)). We will consider this in section 4 when we study the gauge structure for the Lorentzian path integral, where we will see that the gauge freedom allows us to fix $\dot{N} = f(q^A, p_A, N)$.

Fixing for now the gauge as $\dot{N} = 0$, we can canonically quantize the system (22) by replacing:

$$
G^{AB} p_A p_B \longrightarrow -\frac{\hbar^2}{\sqrt{-G}}\partial_A\left(\sqrt{-G}\, G^{AB}\partial_B\right). \qquad (23)
$$

This is the Laplace-Beltrami operator which is a covariant generalisation of the Laplace operator. We see that the replacement (23) requires a choice of factor ordering. The Laplace-Beltrami choice used here ensures invariance of the kinetic term under transformations of the configuration space, but this choice is not unique. Using the above quantization procedure we obtain the Wheeler-de Witt equation as:

$$
\mathcal{H}\Psi = 0 \;\Leftrightarrow\; \frac{1}{2}\left(\frac{\hbar^2}{12\pi^2 a^2}\partial_a(a\partial_a) - \frac{\hbar^2}{2\pi^2 a^3}\partial_\phi^2 + 2\pi^2\left[-6a + 2a^3\Lambda + m^2 a^3 \phi^2\right]\right)\Psi[a,\phi] = 0\,, \qquad (24)
$$

and the Hamiltonian formulation of the action is

$$
S = \int \mathrm{d}t\left[p_A \dot{q}^A - H(p,q)\right] = \int \mathrm{d}t\,\frac{N}{2}\left[-\frac{p_a^2}{12\pi^2 a} + \frac{p_\phi^2}{2\pi^2 a^3} + 2\pi^2\left(6a - 2\Lambda a^3 - m^2 a^3\phi^2\right)\right]. \qquad (25)
$$

Mathematically, the WdW equation is a second order equation for the wavefunction Ψ, which is reminiscent of the Klein-Gordon equation of a scalar field. This is the root of the "problem of time" [32] of canonical quantum gravity: the WdW equation is a constraint equation, rather than a dynamical equation describing an evolution with respect to a specific time parameter. In order to obtain a probabilistic interpretation of quantum cosmology as in non-relativistic quantum mechanic, one must construct a well-defined inner-product. However here the quantity $\Psi\Psi^\star$ cannot serve as a probability measure because it is not normalisable. In analogy with the Klein-Gordon equation, one can instead construct a conserved current

$$
J^A = -\frac{i\hbar}{2}\left(\Psi^\star\nabla^A\Psi - \Psi\nabla^A\Psi^\star\right) \qquad (26)
$$

such that $\nabla_A J^A = 0$, and use the integral of J^0, where the node denotes some timelike direction in minisuperspace, as an inner product, but that is non-positive definite in general.

The interpretation of the wavefunction of the universe Ψ must thus be subject to caution. It has provoked fruitful discussions on the interpretation of quantum mechanics (consistent histories and decoherence versus the standard Copenhagen interpretation [33, 34]), as well as discussions on

PoS(Modave2024)003

the concept of unitarity and time evolution [35–37], [38]. The no-boundary [3, 4] and tunneling [5, 6] proposals that we will discuss in the next section similarly aim to refine the interpretation of the wavefunction of the universe. It is also the same line of thought that later led to the approach of top-down quantum cosmology [39, 40].

2.3 Solutions to the Wheeler-de Witt equation

In the absence of a scalar field, the WdW equation (24) can be solved exactly depending on the boundary conditions chosen for Ψ [41]. The system simplifies drastically if we use another gauge choice (that we will in fact re-use later on in the context of the no-boundary proposal): $N = \tilde{N}/a$. Then the Hamiltonian (22) reads $H(p_a, a) = \tilde{N}\left(-\frac{p_a^2}{24\pi^2 a^2} + 2\pi^2(-3+\Lambda a^2)\right) \equiv \tilde{N}\mathcal{H}$, and $G^{aa} = -1/(12\pi^2 a^2)$. The WdW equation becomes:

$$\mathcal{H}\Psi[a] = \left[\frac{\hbar^2}{24\pi^2 a}\partial_a\left(\frac{1}{a}\partial_a\right) + 2\pi^2(\Lambda a^2 - 3)\right]\Psi[a] = 0\,, \tag{27}$$

whose general solution is

$$\Psi[a] = c_1\,\mathrm{Ai}\left(\frac{(-12\pi^4)^{1/3}(3-a^2\Lambda)}{(\hbar^2\Lambda^2)^{1/3}}\right) + c_2\,\mathrm{Bi}\left(\frac{(-12\pi^4)^{1/3}(3-a^2\Lambda)}{(\hbar^2\Lambda^2)^{1/3}}\right)\,. \tag{28}$$

Ai and Bi are the Airy functions of first and second kind, while c_1 and c_2 are coefficients that are fixed by the boundary conditions. The choice of boundary conditions is related to the interpretation of the solution, for instance the tunneling proposal of Vilenkin [5] sets $c_2 = ic_1$ and so

$$\Psi_{\mathrm{V}}[a] \propto \mathrm{Ai}\left(\frac{(-12\pi^4)^{1/3}(3-a^2\Lambda)}{(\hbar^2\Lambda^2)^{1/3}}\right) + i\,\mathrm{Bi}\left(\frac{(-12\pi^4)^{1/3}(3-a^2\Lambda)}{(\hbar^2\Lambda^2)^{1/3}}\right). \tag{29}$$

This choice of boundary conditions is such that $\lim_{a\to\infty}\Psi[a] = 0$ when $\Lambda < 0$ (in the classically forbidden region at large a when $\Lambda < 0$, the Vilenkin choice picks the decaying branch), in other words, the Vilenkin wavefunction selects the purely outgoing wave in a at large a. This is the so-called "tunneling boundary condition" [18]. For large values of a and positive cosmological constant $\Lambda > 0$, it can be approximated as:

$$\Psi_{\mathrm{V}} \sim \frac{1}{\sqrt{a}}\exp\left(-\frac{12\pi^2}{\hbar\Lambda} - \frac{12\pi^2}{\hbar\Lambda}i\sqrt{\Lambda a^2/3-1}^{\,3}\right). \tag{30}$$

In what follows we will compare the Vilenkin boundary condition with the Hartle-Hawking no-boundary one, where we set $c_2 = 0$, such that

$$\Psi_{\mathrm{HH}}[a] \propto \mathrm{Ai}\left(\frac{(-12\pi^4)^{1/3}(3-a^2\Lambda)}{(\hbar^2\Lambda^2)^{1/3}}\right). \tag{31}$$

In that case the large a approximation gives:

$$\Psi_{\mathrm{HH}} \sim \exp\left(\frac{12\pi^2}{\hbar\Lambda}\right)\cos\left(\frac{12\pi^2}{\hbar\Lambda}\sqrt{\Lambda a^2/3-1}^{\,3} - \pi/4\right). \tag{32}$$

This choice of boundary condition derives from the path integral formulation that we turn to in the next two sections.

PoS(Modave2024)003

3. Path integral quantization and the no-boundary proposal

3.1 Path integral quantization

The path integral quantization was originally proposed by Feynman as an alternative formulation of non-relativistic quantum theory [42]. It constructs the wavefunction of a quantum state as an integral summing over all the possible paths in configuration space linking an initial to a final coordinates position, and weighted by an exponential of the classical action multiplied by a factor i and divided by $\hbar$:

$$\Psi(x_i, t_i; x_f, t_f) = \int_{\{x_i,t_i\}}^{\{x_f,t_f\}} \mathcal{D}x\, e^{iS[x]/\hbar}\,. \tag{33}$$

$\mathcal{D}x$ is a measure on the configuration space, while $S[x]$ is the action evaluated on the coordinates position x. This wavefunction was shown to satisfy the Schrödinger equation, proving the equivalence of this formulation with the more familiar Schrödinger's and Heisenberg's pictures of quantum mechanics. The path integral picture also allows for a straightforward semi-classical limit when $\hbar \to 0$: using the WKB approximation[13], the wavefunction (33) reduces to a sum over the classical, saddle point solutions:

$$\Psi(x_i, t_i; x_f, t_f) \simeq \mathcal{N} \sum_{\substack{\text{saddle}\\ \text{points}}} e^{iS_{\text{on-shell}}[\text{S.P.}]/\hbar}\,. \tag{34}$$

This formulation has been successfully adapted to field theory, where it provided one of the most efficient way of quantizing fields such as Yang-Mills. In this case we write the generating functional of Green's function as the path integral:

$$\mathcal{Z}[J] = \int \mathcal{D}\Phi\, e^{i(S[\Phi]+J_A\Phi^A)/\hbar}\,, \tag{35}$$

with $\mathcal{D}\Phi$ the measure on the fields Φ, and $S[\Phi]$ the action on those fields. $\mathcal{Z}[J]$ thus provides correlation functions and propagators for the field theory in the presence of the source J.

The path integral idea was first generalized to include gravity in [3]. The gravitational case is far from a simple continuation from the field theory one. In terms of definition though, the only difference is that the gravitational path integral also sums over the metric configurations in addition to the sum over matter fields. The amplitude of probability to go from a state with metric g_1 and matter field Φ_1 at time t_1, to a second state with metric g_2 and matter fields Φ_2 at time t_2 is then given by:

$$\langle g_1, \Phi_1, t_1 | g_2, \Phi_2, t_2 \rangle = \int \mathcal{D}g\, \mathcal{D}\Phi\, e^{iS[g,\Phi]/\hbar}\,, \tag{36}$$

where the path integral sums over all field configurations, including the metric, with the appropriate initial and final values. This provides another way to construct the wavefunction of the universe, which must be a solution to the WdW equation (17), as we will explicitly show later on for the specific case of the no-boundary wavefunction.

[13] Developed in 1926 by Wentzel, Kramer and Brillouin, the WKB approximation is a method for approximating solutions to linear differential equations such as the Schrödinger's equation, valid when the amplitude of the wavefunction varies slowly compared to its phase.

PoS(Modave2024)003

From a quantum mechanical perspective, the inclusion of gravity in the path integral is a natural extension, because spacetime is always deformed (although very weakly) by the presence of a particle here or there. In that sense the full path integral must also sum over different spacetime configurations, but the weakness of the gravitational interaction with respect to the other forces allows us to neglect it for non-Planckian energies and small curvature spaces.

We will distinguish the **Euclidean path integral formulation**, which computes the partition function

$$\mathcal{Z}_{\text{grav}} = \int \mathcal{D}g\mathcal{D}\Phi\, e^{-\mathcal{I}_{\text{E}}[g,\Phi]}\,, \tag{37}$$

based on the Euclidean action $\mathcal{I}_{\text{E}}[g,\Phi]$ of both the metric g and the matter fields Φ, from the **Lorentzian path integral formulation**, which computes the wavefunction (solution to the associated WdW equation)

$$\Psi = \int \mathcal{D}g\mathcal{D}\Phi\, e^{iS[g,\Phi]/\hbar}\,, \tag{38}$$

using $S[g,\Phi]$, the Lorentzian action of the metric g and the matter fields Φ.

These formal definitions will be applied in the context of the no-boundary proposal to which we turn now.

3.2 The no-boundary proposal and the Euclidean path integral

As reviewed in section 1, the hot big bang model based on the FLRW metric is a very faithful description of our early universe. It is often supplemented by an earlier inflationary phase where the scale factor grows exponentially, resolving issues with causality and extreme flatness observed in the CMB. However this model doesn't provide initial conditions to the early universe. In particular, the big bang model, with or without inflation, leads to a geodesically incomplete spacetime [43]. This renders the existence of an initial singularity in Lorentzian spacetime unavoidable, and leads to the necessity of a "quantum beginning of spacetime". The question of finding initial conditions for our universe is therefore intrinsically a quantum gravity question.

The no-boundary proposal of Hartle and Hawking suggests to answer this question by stating that the quantum state of (a spatially closed) universe is given by the Euclidean path integral summing over all compact and regular geometries with only one final hypersurface boundary. In other words, the partition function[14] of the universe is found by summing over all geometries that have no boundary in the past:

$$\mathcal{Z}[\gamma_{ij}^{\text{final}}, \Phi_{\text{final}}] = \int_{\mathcal{M}} \mathcal{D}g\mathcal{D}\Phi\, e^{-\mathcal{I}_{\text{E}}[g,\Phi]/\hbar}\,. \tag{39}$$

$\mathcal{M}$ is the set of all possible four-geometries that possess only one final boundary, the three-dimensional hypersurface $\gamma_{ij}^{\text{final}}$. The matter fields Φ take values Φ_{final} on that final hypersurface. The geometries in $\mathcal{M}$ must necessarily be complex, since purely Lorentzian spacetimes cannot be

[14]Often we will loosely talk about the wavefunction of the universe, whichever formulation of the path integral is used, as the two formulations can be related to each other by transforming the Euclidean into the Lorentzian action upon using a Wick rotation for the time integral: $\mathcal{I}_{\text{E}} \equiv -iS$.

PoS(Modave2024)003

both compact and non-singular[15]. This definition is very general but in practice its implementation faces many obstacles. The first is the number of degrees of freedom we are dealing with: the metric corresponds to 10 fields all depending on space and time coordinates. So far the only known way of dealing with that is to reduce this number by more or less justified approximations. A second problem is that these fields are highly constrained by diffeomorphism invariance: the sum over geometries must only include independent geometries, so gauge redundancy must be eliminated. This will be done using the BRST technique and we will see how it works in the next section.

Another problem lies in the use of the Euclidean path integral itself in the presence of gravity. This can already be exemplified in the simplest case. Consider a Euclidean metric with the scale factor as unique degree of freedom in a spatially closed space ($k = 1$): $\mathrm{d}s^2 = N(\tau)^2\mathrm{d}\tau^2 + a(\tau)^2\mathrm{d}\Omega_3^2$. We take as matter content a homogeneous massless scalar field $\phi(\tau)$. The total Euclidean action then reads

$$\mathcal{I}_\mathrm{E}[g_{\mu\nu},\phi] = -\frac{1}{2}\int \mathrm{d}^4x\sqrt{g}\,(R-2\Lambda) - \int_{\partial\mathcal{M}} \mathrm{d}^3y\sqrt{h}\,K + \frac{1}{2}\int \mathrm{d}^4x\sqrt{g}\,\partial_\mu\phi\partial^\mu\phi\,, \tag{40}$$

$$= 2\pi^2\int \mathrm{d}\tau\,\left[-\frac{3aa'^2}{N} + a^3N\Lambda - 3aN + \frac{a^3\phi'^2}{2N}\right]. \tag{41}$$

We still can ignore the boundary terms at this point and will consider them when we study saddle point solutions later on.

From (41), it is apparent that the kinetic term associated with the scale factor has the wrong sign compared to the sign of the scalar field kinetic term. Therefore the integrand of the Euclidean path integral is unbounded from below[16], casting doubts on its physical meaning.

These hurdles are what motivates the Lorentzian path integral formulation. The Lorentzian path integral removes the conformal mode problem by introducing conditionally convergent integrals, which can be unambiguously defined through the Picard-Lefschetz method. This will be the topic of the next section.

Before that, we will study the classical solutions to the equations of motion in the minisuperspace context and obtain the saddle point approximation to the no-boundary wavefunction.

3.3 Saddle point solutions

For a practical implementation of the no-boundary proposal we restrict to minisuperspace with a spatially close slicing $k = 1$: $\mathrm{d}s^2 = N^2\mathrm{d}\tau^2 + a(\tau)^2\mathrm{d}\Omega_3^2$. τ is the Euclidean time and the Euclidean action is (we include a GHY term on the final boundary at $\tau_\mathrm{f} = 0$ but not on the initial one since we

[15] Actually from a quantum perspective, hence when performing a path integral for instance, we can never have both compactness (condition on the scale factor a) and regularity (condition on its momentum p through regularity of the Friedman constraint equation) imposed at the same time, as this would contradict the Heisenberg's uncertainty principle. Instead we must make a choice of fixing either the scale factor or the momentum for the path integral (so for off-shell configurations). Those on-shell configurations correspond to classical solutions to the equations of motion (saddle points of the action) and those can be both compact and regular. The usual choice of the no-boundary proposal is to fix the scale factor $a(t = 0) = 0$ where $t = 0$ is the South Pole of the instanton solution.

[16] Another way to see this problem is to consider a conformal transformation $\tilde{g}_{\mu\nu} = \Omega(x^\mu)^2 g_{\mu\nu}$. The Ricci scalar then transforms as $\tilde{R} = \Omega^{-2}R - 6\Omega^{-3}\Box\Omega$, so that we can make the Euclidean action $\mathcal{I}_\mathrm{E}$ as negative as we want by using a rapidly varying conformal factor $\Omega(x^\mu)$: the Euclidean action is unbounded from below.

PoS(Modave2024)003

want to impose the “no-boundary” boundary condition):

$$\mathcal{I}_{\rm E}[g_{\mu\nu}] = -\frac{1}{2}\int \mathrm{d}^4x\sqrt{g_{\rm E}}\,(R-2\Lambda) + \int_{\tau=\tau_{\rm f}} \mathrm{d}^3y\,\sqrt{h}\,K\,, \tag{42}$$

$$= 6\pi^2\int_0^{\tau_f}\mathrm{d}\tau\, aN\left[-\frac{a'^2}{N^2}+\frac{a^2\Lambda}{3}-1\right] - 2\pi^2\left[\frac{3a^2a'}{N}\right]^0, \tag{43}$$

leading to the equations of motion:

$$\begin{cases} -a'^2 + N^2 = \dfrac{\Lambda}{3}a^2N^2\,,\\ 2aa'' + a'^2 + N^2(a^2\Lambda - 1) = 0\,. \end{cases} \tag{44}$$

The solutions to these classical equations of motion are the **saddle point solutions** of the Euclidean path integral, sometimes called *instantons*. One typical instance of such an instanton is depicted in figure 4. It consists of a four-dimensional de Sitter hyperboloid (dS_4) glued at its waist onto the equator of a lower-half four-sphere (S^4). The metrics are given by the line elements

$$\mathrm{d}s^2_{S^4} = N^2\mathrm{d}\tau^2 + \frac{\sin^2(H\cdot N\tau)}{H^2}\mathrm{d}\Omega^2_{(3)}\,, \tag{45a}$$

$$\mathrm{d}s^2_{\mathrm{dS}_4} = -N^2\mathrm{d}t^2 + \frac{\cosh^2(H\cdot Nt)}{H^2}\mathrm{d}\Omega^2_{(3)}\,, \tag{45b}$$

where $\mathrm{d}\Omega^2_{(3)}$ is the metric on a three-sphere of constant radius $1/H$, and the two metrics are related to each other through a Wick rotation:

$$t = -i\left(\tau - \frac{\pi}{2H}\right)\,. \tag{46}$$

Realistic instantons have a completely regular geometry and do not present such a sharp change of signature from Euclidean to Lorentzian, which would otherwise induce a discontinuity. These are then fully complex and sometimes called *fuzzy instantons* [44], as shown by the light orange line on the right of figure 4. Note that this saddle point solution is such that the boundary term present in (43) automatically vanishes.

In the semi-classical limit, the path integral is evaluated by summing over all relevant saddle point solutions, leading to a definite expression for the wavefunction of a closed universe at the semi-classical level:

$$\Psi[a_{\rm f},\tau_{\rm f}] = \mathcal{N}\sum_{\substack{\text{relevant}\\ \text{saddle points}}} e^{-\mathcal{I}_{\rm E}[\text{saddle point}]/\hbar} + O(\hbar)\,, \tag{47}$$

where $\mathcal{N}$ is some weighting not important for this discussion. Saddle point values of the lapse, denoted N_σ, are found as solutions to the saddle point equation:

$$\left.\frac{\partial\mathcal{I}_{\rm E}^{\text{on-shell}}}{\partial N}\right|_{N_\sigma} = 0\,, \tag{48}$$

PoS(Modave2024)003

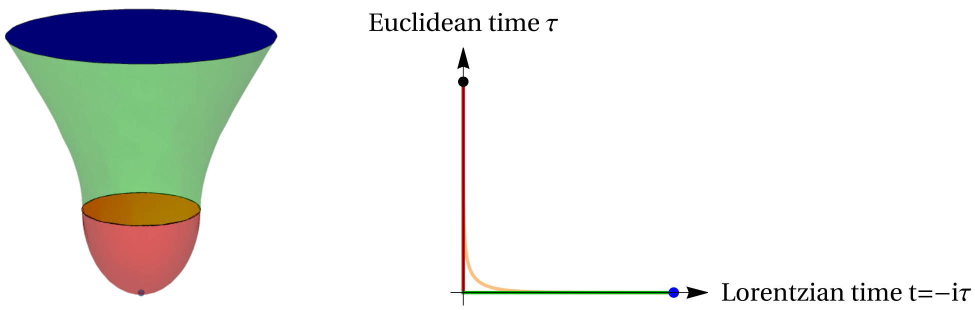

Figure 4: *Left:* Pictorial representation of an instanton: no-boundary geometry consisting in the gluing of a lower-half four-sphere (Euclidean solution, in red (45a)) onto the waist of the hyperboloid of a four-dimensional de Sitter (dS) space (Lorentzian solution, in green (45b)). This does not represent an evolution in time but instead one instanton geometry. Only the final upper hypersurface (in blue) is classical and has real field values. The real time evolution is given by a succession of such geometries, with larger and larger final hypersurfaces. *Right:* Contour in the complex time plane associated with the instanton geometry depicted to the left. We start from a purely Euclidean space at the South Pole of the instanton, and end in the purely Lorentzian direction on the final real hypersurface. Fuzzy instantons corresponding to more realistic geometries avoid the origin of the plot and describe a fully complex geometry as the light orange line suggests.

where $\mathcal{I}_{\mathrm{E}}^{\text{on-shell}}$ is the Euclidean Einstein-Hilbert action (43) evaluated on the classical solutions to the equations of motion (45a). At background level for the pure gravity case, we find (using that $\Lambda/3 = H^2$ from the constraint equation (44)):

$$\mathcal{I}_{\mathrm{E}}^{\text{on-shell}} = 6\pi^2 \int_0^{\tau_{\mathrm{f}}} \mathrm{d}\tau \frac{N}{H} \sin(HN\tau) \left[-\cos^2(HN\tau) + \frac{\Lambda}{3H^2} \sin^2(HN\tau) - 1 \right], \tag{49}$$

$$= -12\pi^2 \int_0^{\tau_{\mathrm{f}}} \mathrm{d}\tau \frac{N}{H} \sin(HN\tau)\cos^2(HN\tau) = -12\pi^2 \left[-\frac{1}{3H^2} \cos^3(HN\tau) \right]_0^{\tau_{\mathrm{f}}}, \tag{50}$$

$$= \frac{4\pi^2}{H^2} \left(\cos^3(HN\tau_{\mathrm{f}}) - 1 \right) \equiv -\frac{4\pi^2}{H^2} \left(1 \mp i \sqrt{a_{\mathrm{f}}^2 H^2 - 1}^{\,3} \right), \tag{51}$$

where for the last equality we used

$$\tau_{\mathrm{f}} = \frac{\pi}{2H} \pm i t_{\mathrm{f}} \quad \text{and} \quad a_{\mathrm{f}} \equiv a(t_{\mathrm{f}}) = \frac{\cosh(HN_\sigma t_{\mathrm{f}})}{H}. \tag{52}$$

Therefore

$$\left. \frac{\partial \mathcal{I}_{\mathrm{E}}^{\text{on-shell}}}{\partial N} \right|_{N_\sigma} = -\frac{12\pi^2}{H} \tau_{\mathrm{f}} \sin(HN_\sigma \tau_{\mathrm{f}}) \cos^2(HN_\sigma \tau_{\mathrm{f}}) = 0 \;\Rightarrow\; N_\sigma = \pm \frac{1 \mp i \cdot 2Ht_{\mathrm{f}}/\pi}{1 + 4H^2 t_{\mathrm{f}}^2/\pi^2}. \tag{53}$$

This gives us four saddle points (we've excluded $N_\sigma = 0$ because that corresponds to an unphysical interval $\mathrm{d}s^2$), related by time reversal and complex conjugation. The four saddles are represented schematically for any $t_{\mathrm{f}} > 0$ in Fig. 5. The blue sign choice follows from the choice of Wick rotation's direction. In particular, the positive (resp. negative) sign for the rotation (i.e., negative (resp. positive) imaginary part for the saddle point) is associated with the Hartle-Hawking (resp. Vilenkin) choice.

The whole crux of the debate from this point onward is then: which of these saddles are the "relevant" one that must be included in the sum (47)?

PoS(Modave2024)003

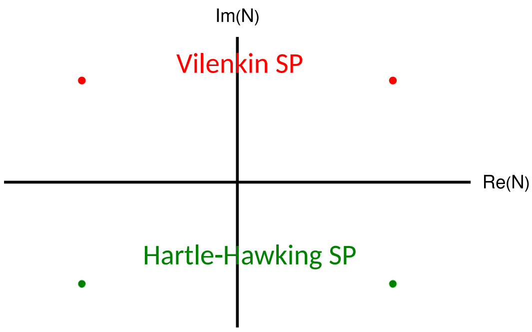

Figure 5: Schematic position in the complex lapse plane of the four saddle points of pure gravity in the regime where $t_{\mathrm{f}} > 0$ (Lorentzian regime).

One approach is to refer to some symmetry argument: for instance that the saddle points chosen must be those that lead to the Vilenkin wavefunction (29) in order to get only out-going modes at the origin. Another choice is to select the saddles describing geometries which are stable with respect to fluctuations of spacetime (i.e., when considering perturbations on top of the background geometry, these perturbations are exponentially suppressed and not enhanced (see e.g. [45]). This selects the two Hartle-Hawking saddle points, and the associated Hartle Hawking wavefunction (31).

However as shown at the end of the last subsection, the Euclidean path integral formulation suffers from the conformal mode problem. We next turn to the Lorentzian path integral formulation to see how it can resolve this problem and automatically select specific saddle points. We will find two possibilities which are associated with different interpretations but also different complications.

3.4 From Euclidean to Lorentzian

Before we continue with the Lorentzian formulation of the path integral for gravity, let us quickly recall the link between the Euclidean and Lorentzian action to avoid any confusion. After performing a Wick-rotation, the Euclidean and Lorentzian path integral should be equivalent. Therefore we have (using $K_{\mathrm{L}} = -h^{ij}\dfrac{\partial_t h_{ij}}{2N}$ and $K_{\mathrm{E}} = -h^{ij}\dfrac{\partial_\tau h_{ij}}{2N}$)

$$iS_{\mathrm{L}} \equiv -\mathcal{I}_{\mathrm{E}}\,, \tag{54}$$

$$\begin{aligned}
\Leftrightarrow\; i\int \mathrm{d}^3x\mathrm{d}t\sqrt{-g}\left(\frac{R}{2}-\Lambda\right) + i\int \mathrm{d}^3y\sqrt{h}\,K_{\mathrm{L}} &= \int \mathrm{d}^3x\mathrm{d}\tau\sqrt{g_{\mathrm{E}}}\left(\frac{R}{2}-\Lambda\right) - \int \mathrm{d}^3y\sqrt{h}\,K_{\mathrm{E}}\,,\\
\Leftrightarrow\; i\cdot 2\pi^2\int_0^{t_{\mathrm{f}}}\mathrm{d}t\,N\left(-\frac{3a\dot{a}^2}{N^2}+3a-a^3\Lambda\right) &= 2\pi^2\int_0^{\tau_{\mathrm{f}}}\mathrm{d}\tau\,N\left(\frac{3aa'^2}{N^2}+3a-a^3\Lambda\right).
\end{aligned} \tag{55}$$

The last equality indeed holds for the Wick rotation $\mathrm{d}t = -i\mathrm{d}\tau$.

4. Lorentzian path integral and the Picard-Lefschetz theory

Now that the general context of the no-boundary proposal has been set up and that we have encountered the hinders of using the Euclidean gravitational path integral, we will study how the Lorentzian gravitational path integral behaves.

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The first step is to understand how the path integral over the geometry g reduces in the context of minisuperspace to a simple path integral over the scale factor a and a normal integral over the lapse function N. To do so we must first deal with the gauge redundancies inherent to general relativity. In the presence of gauge symmetries, the path integral quantization must be performed modulo the gauge transformation, so if the gauge group is G, we need to integrate on:

$$\int_{\mathcal{M}/G} \mathcal{D}g\, e^{iS[g]/\hbar} . \tag{56}$$

But in practice it will be easier to first pick a gauge and then integrate only on geometries that satisfy the gauge condition:

$$\int_{\mathcal{M}|\text{gauge condition}} \mathcal{D}g\, e^{iS[g]/\hbar} . \tag{57}$$

In order to make sure that we do not pick up some Jacobian factor going from (56) to (57), we will use the BRST procedure due to Becchi, Rouet, Stora and Tyurin. This will necessitate the introduction of additional ghost fields and the use of a new symmetry, the BRST symmetry. We will follow this procedure directly for the time reparametrisation invariance of GR, but this is applicable to any gauge invariance and one easy and common example to get intuition from is to apply this procedure on the $U(1)$ gauge symmetry of QED (see for instance Hugh Osborn's Advanced Quantum Field Theory lecture notes, subsection 5.7).

After that we will finally have to perform the scale factor and lapse integrals. The scale factor path integral will reduce to a Gaussian integral in our simple toy-model, that we can integrate right away. For the lapse integral, we will have to deal with a highly oscillating integral, and this is where the Picard-Lefschetz method will come at hand.

4.1 Lorentzian path integral using BRST

We have seen in the canonical formulation that the gravitational action is schematically

$$S_g = \int \mathrm{d}t \left(p_A \dot{q}^A - N\mathcal{H} \right) , \tag{58}$$

where $\mathcal{H} = \frac{p_A^2}{2} + V(q)$. We will focus on the time reparametrisation invariance because this is really the conceptual difference between gravitational systems and other gauge-invariant systems such as Yang-Mills or QED. For the purpose of these notes it is sufficient to work in the minisuperspace Lorentzian metric (although a full generalisation is possible, see [41])

$$\mathrm{d}s^2 = -N(t)^2 \mathrm{d}t^2 + a(t)^2 \mathrm{d}\Omega_3^2 . \tag{59}$$

One can show [46] that an admissible gauge condition must be of the form

$$\dot{N} = f(a, p, N) , \tag{60}$$

with no explicit dependence on time.

This is valid for any Hamiltonian system with a quadratic constraint:

$$S = \int_{t_i}^{t_f} \mathrm{d}t (p\dot{a} - N\mathcal{H}) , \quad \text{with} \quad \mathcal{H} = p^2 + V(a) . \tag{61}$$

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Indeed if we consider an infinitesimal time reparametrisation $t \longrightarrow t + \epsilon(t)$, then the transformation:

$$\delta_\epsilon a = \epsilon\{a, \mathcal{H}\}\,, \quad \delta_\epsilon p = \epsilon\{p, \mathcal{H}\}\,, \quad \delta_\epsilon N = \dot{\epsilon}\,, \tag{62}$$

leaves the action S invariant up to a boundary term:

$$\delta_\epsilon S = \left[\epsilon\left(p\frac{\partial \mathcal{H}}{\partial p} - \mathcal{H}\right)\right]_{t_i}^{t_f}\,. \tag{63}$$

However since the constraint is quadratic and not linear, this boundary term vanishes only if $\epsilon(t_f) = 0 = \epsilon(t_i)$. This means that there is no gauge freedom at the end points, and therefore usual choices of canonical gauge of the form $t = \phi(a, p)$ are over-restrictive because they also fix end points. Instead the gauge condition must be such that:

1. any starting history can always be deformed into one where the gauge condition holds using only iterative transformations (62);

2. the gauge must be fixed completely, meaning that the only transformation (62) that preserves the gauge condition is when $\epsilon(t) = 0$.

These two conditions are satisfied if and only if applying a gauge transformation (62) to the gauge condition itself yields a second-order differential operator on ϵ with a unique inverse given the boundary conditions $\epsilon(t_f) = 0 = \epsilon(t_i)$. The existence of the inverse ensures point 1 while its uniqueness ensures point 2. Given the form of the gauge transformation, an admissible gauge condition must be of the form $F(\dot{N}, a, p, N) = 0$, and in particular a wide class of such admissible gauge condition is given by (60).

This can be implemented as a constraint in the action by adding the gauge-fixing term:

$$S_{\text{gf}} = \int \mathrm{d}t\, \Pi(\dot{N} - f)\,, \tag{64}$$

where Π is the conjugate momentum of the lapse. The next step is to make sure that the path integral is independent on the choice of f. This is done by adding Fadeev-Popov anticommuting ghost fields C, $\bar{C}$ (with momenta P, $\bar{P}$) with a specific ghost action:

$$S_{\text{ghost}} = \int \mathrm{d}t\, \left[\bar{P}\dot{C} + \bar{C}\dot{P} - \bar{P}P + C\,\{f, \mathcal{H}\}\,\bar{C} + P\frac{\partial f}{\partial N}\bar{C}\right]\,, \tag{65}$$

where $\{f, \mathcal{H}\} = \frac{\partial f}{\partial a}\frac{\partial \mathcal{H}}{\partial p} - \frac{\partial \mathcal{H}}{\partial a}\frac{\partial f}{\partial p}$ is the Poisson bracket. One can show that the total action $S_{\text{tot}} = S_g + S_{\text{gf}} + S_{\text{ghost}}$ possesses an additional symmetry (the BRST symmetry):

$$\delta a = \epsilon \cdot C\frac{\partial \mathcal{H}}{\partial p}\,,\ \delta p = -\epsilon \cdot C\frac{\partial \mathcal{H}}{\partial a}\,,\ \delta N = \epsilon \cdot P\,, \tag{66}$$

$$\delta\Pi = \delta C = \delta P = 0\,,\ \delta\bar{C} = -\epsilon \cdot \Pi\,,\ \delta\bar{P} = -\epsilon \cdot \mathcal{H}\,, \tag{67}$$

where ϵ is an anticommuting Grassmann number and with boundary conditions such that Π, C and $\bar{C}$ vanish at the end points. Then one can construct the path integral with Liouville measure:

$$\Psi = \int \mathcal{D}a\mathcal{D}p\mathcal{D}N\mathcal{D}\Pi\mathcal{D}C\mathcal{D}\bar{C}\mathcal{D}P\mathcal{D}\bar{P}\, e^{\frac{i}{\hbar}S_{\text{tot}}}\,. \tag{68}$$

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By construction this is BRST-invariant for any parameter ϵ, and in particular if we choose the parameter

$$\epsilon = \frac{i}{\hbar}\int \mathrm{d}t\, \bar{C}(f - \tilde{f})\,, \tag{69}$$

then the Jacobian of this transformation effectively replaces f by $\tilde{f}$ in the ghost action:

$$\mathrm{Jac} = e^{\frac{i}{\hbar}\int \mathrm{d}t \left(C\{\tilde{f}-f,\mathcal{H}\}\bar{C} + P\frac{\partial(\tilde{f}-f)}{\partial N}\bar{C}\right)}\,. \tag{70}$$

This means that the path integral is independent on the choice of f so we can choose $f = 0$ or more complicated functions. For instance, the choice of metric $\mathrm{d}s^2 = -\left(N^2/q(t)\right)\mathrm{d}t^2 + q(t)\mathrm{d}\Omega_3^2$ with $\dot{N} = 0$, that is very often used in quantum cosmology, implies that $f \propto N^2 p/q^2 = \tilde{N}^2 p/q$, with $\tilde{N} = N/\sqrt{q}$.

Focusing on the choice $f = 0$ for now, the path integral over the ghosts decouples from the other fields so it only gives a numerical factor in the path integral,

$$\int \mathcal{D}C\mathcal{D}\bar{C}\mathcal{D}P\mathcal{D}\bar{P}\exp\!\left(\frac{i}{\hbar}\int \mathrm{d}t\,\left[\bar{P}\dot{C} + \bar{C}\dot{P} - \bar{P}P\right]\right) = 1\,, \tag{71}$$

since the ghost fields vanish at the end points. The lapse momentum Π only appears in the gauge-fixing action, so its path integral can be performed directly to give:

$$\Psi = \int \mathcal{D}a\mathcal{D}p\mathcal{D}N\, e^{iS_g[N,a,p]}\int \mathcal{D}\Pi\, e^{\frac{i}{\hbar}\int \mathrm{d}t\,\Pi\dot{N}} \tag{72}$$

$$= \int \mathcal{D}a\mathcal{D}p\, \mathrm{d}N_1\cdots \mathrm{d}N_{n+1}\, e^{\frac{i}{\hbar}S_g[N,a,p]}\frac{1}{(2\pi)^n}\int \mathrm{d}\Pi_1\cdots \mathrm{d}\Pi_n\, e^{\frac{i}{\hbar}\sum_{k=1}^{n}\Pi_k(N_{k+1}-N_k)} \tag{73}$$

$$= \int \mathcal{D}a\mathcal{D}p\, \mathrm{d}N_1\cdots \mathrm{d}N_{n+1}\, e^{\frac{i}{\hbar}S_g[N,a,p]}\prod_{k=1}^{n}\delta(N_{k+1}-N_k) = \int \mathcal{D}a\mathcal{D}p\,\mathrm{d}N_1\, e^{\frac{i}{\hbar}S_g[N_1,a,p]}\,, \tag{74}$$

where we have used that $\Pi_0 = \Pi_{n+1} = 0$.

4.2 Oscillating integrals using Picard Lefschetz theory

At this point we have expressed the Lorentzian path integral for gravity with no gauge invariance left and we obtained:

$$\Psi = \int \mathcal{D}a\mathcal{D}p\,\mathrm{d}N\exp\!\left(\frac{i}{\hbar}S_g[N,a,p]\right). \tag{75}$$

We expand the scale factor a and momentum $p^{(a)}$ around the classical solutions to the equations of motion as $a = a_{\mathrm{cl}} + \mathcal{A}$ and $p^{(a)} = p^{(a)}_{\mathrm{cl}} + \mathcal{P}^{(a)}$. We can then expand the action at quadratic order around the classical solutions (the linear term vanishes thanks to the equations of motion)

$$S[a,p,N] = S_0[a_{\mathrm{cl}}, p^{(a)}_{\mathrm{cl}}, N] + S_2[\mathcal{A},\mathcal{P}^{(a)},N]\,. \tag{76}$$

The path integral then becomes

$$\Psi = \int \mathrm{d}N\, e^{\frac{i}{\hbar}S_0[a_{\mathrm{cl}},\, p^{(a)}_{\mathrm{cl}},\, N]}\int \mathcal{D}\mathcal{A}\,\mathcal{D}\mathcal{P}^{(a)}\, e^{\frac{i}{\hbar}S_2[\mathcal{A},\,\mathcal{P}^{(a)},\,N]}\,. \tag{77}$$

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The integrals over $\mathcal{P}^{(a)}$ and $\mathcal{A}$ are fluctuation integrals yielding a factor N^{α}, with an exponent depending on the boundary conditions. We will calculate it for specific examples in the next subsection.

The final step is to evaluate the oscillating integral over the lapse function,

$$\int \mathrm{d}N\, e^{\frac{i}{\hbar}S_0[a_{\rm cl},\, p_{\rm cl}^{(a)},\, N]}\,. \tag{78}$$

There are several ambiguities hidden inside this formula. The first concerns the domain of integration of the lapse function. Depending on the choice $N \in (-\infty, +\infty)$, $N \in (0, +\infty)$ or any other initial complex contour, one effectively selects different initial conditions for the quantum state of the universe (Hartle-Hawking, Vilenkin, etc.). Further, the function $S_0[N]$ may possess singularities in the complex plane that must be bypassed, leading to different choices and yet different definitions. Finally, any oscillating integral of the form:

$$I = \int_C \mathrm{d}x\, e^{iS[x]/\hbar}\,, \tag{79}$$

(where $S[x]$ is real, $\hbar$ is a real (small) parameter and C is a domain of integration in $\mathbb{R}$) is only conditionally convergent because the integrand modulus is equal to 1. This last ambiguity can be resolved using Picard-Lefschetz theory, which enables us to rewrite conditionally convergent integrals as a sum of absolutely convergent integrals when it is possible, and also tells us when this is not possible. We will present this method in the rest of this subsection.

Picard-Lefschetz method First we start by extending the integral domain to complex space, $x \in \mathbb{C}$, which turns the function $S[x]$ into a holomorphic function. For convenience we write $x = u^{(1)} + iu^{(2)}$ with $u^{(1,2)} \in \mathbb{R}$. The aim will be to deform the contour C using Cauchy's theorem into a complex contour such that the integral I becomes manifestly convergent. Ideally, we want to deform C into steepest descent contours, also called Lefschetz thimbles, which are the contours along which the function $S[x]$ decreases the fastest, and will therefore necessarily make the integral I converge. More concretely, we rewrite

$$iS[x]/\hbar \equiv W[x] + iP[x], \tag{80}$$

$W[x]$ is the weighting and $P[x]$ is the phase. Then we define **downward flows** $\mathcal{J}$ by the equation

$$\frac{\mathrm{d}u^{(i)}}{\mathrm{d}\lambda} = -g^{ij}\frac{\partial W}{\partial u^{(j)}}\,, \tag{81}$$

where g_{ij} is a Riemannian metric (that we can take to be Cartesian) and λ is some parameter along $\mathcal{J}$. This flow has two properties:

1. **the weighting W is always decreasing along $\mathcal{J}$: $\frac{\mathrm{d}W}{\mathrm{d}\lambda} < 0$.**
   This can be seen directly by performing the total derivative:

$$\frac{\mathrm{d}W}{\mathrm{d}\lambda} = \sum_i \frac{\partial W}{\partial u^{(i)}}\frac{\mathrm{d}u^{(i)}}{\mathrm{d}\lambda} = -\sum_{i,j} g^{ij}\frac{\partial W}{\partial u^{(i)}}\frac{\partial W}{\partial u^{(j)}} = -\sum_i \left(\frac{\partial W}{\partial u^{(i)}}\right)^2 < 0\,. \tag{82}$$

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2. **the phase P is always constant along $\mathcal{J}$: $\frac{dP}{d\lambda} = 0$.**
   Indeed, by changing variables to $(u, \bar{u}) = (u^{(1)} + iu(2), u(1) - iu^{(2)})$, we find that $g_{uu} = g_{\bar{u}\bar{u}} = 0$ and $g_{u\bar{u}} = 1/2$. Then

$$\frac{du}{d\lambda} = -g^{u\bar{u}} \frac{\partial W}{\partial \bar{u}} \quad \text{and} \quad \frac{d\bar{u}}{d\lambda} = -g^{\bar{u}u} \frac{\partial W}{\partial u} . \tag{83}$$

   Since S is a holomorphic function, we have that

$$\frac{\partial W}{\partial u} = i \frac{\partial P}{\partial u} \quad \text{and} \quad \frac{\partial W}{\partial \bar{u}} = -i \frac{\partial P}{\partial \bar{u}} . \tag{84}$$

   Putting these altogether we find that

$$\frac{dP}{d\lambda} = \frac{\partial P}{\partial u} \frac{du}{d\lambda} + \frac{\partial P}{\partial \bar{u}} \frac{d\bar{u}}{d\lambda} = 2i \frac{\partial P}{\partial u} \frac{\partial P}{\partial \bar{u}} - 2i \frac{\partial P}{\partial \bar{u}} \frac{\partial P}{\partial u} = 0 . \tag{85}$$

Similarly we define **upward flows** $\mathcal{K}$ by the equation

$$\frac{du^{(i)}}{d\lambda} = +g^{ij} \frac{\partial W}{\partial u^{(j)}} , \tag{86}$$

so that along this flow the weighting is now always increasing but the phase is still always constant. Since the phase is constant along these flows, it means that the integral I doesn't oscillate:

$$\left| \int_{\mathcal{J}, \mathcal{K}} dx \, e^{i/\hbar S[x]} \right| \leq \int_{\mathcal{J}, \mathcal{K}} |dx| \left| e^{i/\hbar S[x]} \right| = \int_{\mathcal{J}, \mathcal{K}} |dx| e^{W(x)} . \tag{87}$$

Now we consider the downward and upward flows that passes through **saddle points of the function** $S[x]$, that is points x_σ such that $\left.\frac{\delta S[x]}{\delta x}\right|_{x_\sigma} = 0$ (x_σ are classical solutions to the equations of motion when $S[x]$ is an action as in our case). Then the downward flow $\mathcal{J}_\sigma$ associated with the saddle point x_σ is by definition the steepest descent contour or thimble, while the upward flow $\mathcal{K}_\sigma$ is the steepest ascent contour. The steepest descent and ascent contours associated with one saddle point only intersect at the saddle point itself and do not intersect with each other[17]:

$$\mathcal{J}_\sigma \cap \mathcal{K}_{\sigma'} = \delta_{\sigma\sigma'} . \tag{88}$$

Numerically we can easily find $\mathcal{J}_\sigma$ and $\mathcal{K}_\sigma$ by finding the locii of points with the same phase $P[x_\sigma]$ and we can compute the integral along the steepest descent contours as

$$\int_{\mathcal{J}_\sigma} dx \, e^{i/\hbar S[x]} = e^{iP[x_\sigma]} \int_{\mathcal{J}_\sigma} dx \, e^{W[x]} . \tag{89}$$

The last remaining integral can be computed exactly in some cases, or one can expand in the small parameter $\hbar$ to find the semi-classical saddle point approximation:

$$\int_{\mathcal{J}_\sigma} dx \, e^{W[x]} = e^{W[x_\sigma]} \left(A_\sigma + O(\hbar) \right) . \tag{90}$$

[17]At least in the absence of Stokes phenomena: it may happen that the steepest descent of one saddle point is simultaneously the steepest ascent of another saddle point. This leads to an ambiguity that must be treated for instance by deforming the contours with small parameters.

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The last step is now to determine which saddle points are contributing to the integral I over the contour C, which means that we want to determine the number n_σ such that

$$C = \sum_\sigma n_\sigma \mathcal{J}_\sigma \,. \tag{91}$$

But we can actually use equation (88) and we find that

$$n_\sigma = C \cap \mathcal{K}_\sigma \,, \tag{92}$$

which means that the saddle point x_σ will contribute as many times as its steepest ascent contour intersects the original contour of integration C.

Finally putting all the pieces together, we can calculate the integral I as

$$I = \int_C \mathrm{d}x \, e^{i/\hbar S[x]} = \sum_\sigma n_\sigma \int_{\mathcal{J}_\sigma} \mathrm{d}x \, e^{i/\hbar S[x]} = \sum_\sigma n_\sigma \, e^{i/\hbar S[x_\sigma]} (A_\sigma + O(\hbar)) \,. \tag{93}$$

An important remark is that this procedure only holds when there is no singularity that should be crossed by the contour of integration through its deformation. Figure 6 gives the generic structure of the thimbles and a visual explanation of the above text.

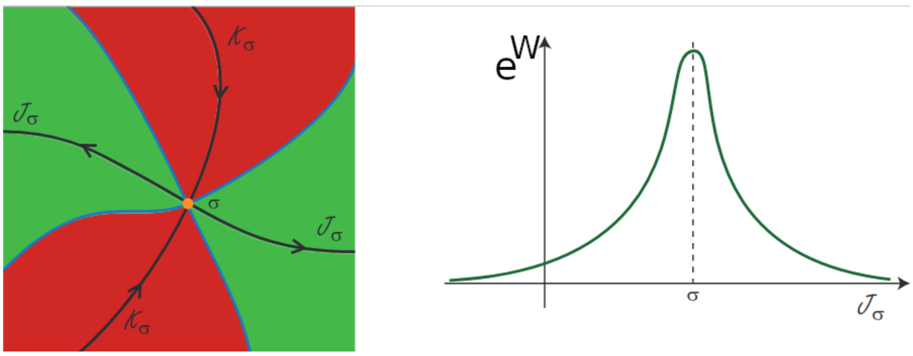

Figure 6: Figures taken from [47]. Left: Generic thimble structure in complex plane around a saddle point σ. Green regions have a weighting W smaller than the saddle point $W[\sigma]$ and red regions have a weighting larger than the saddle point one. The steepest descent and ascent contours in black are the locii of constant phase $P[\sigma]$. The arrows indicate the direction of decreasing weighting. Right: Profile of the weight e^W along a Lefschetz thimble. The main contribution comes from the saddle point and the function is rapidly decreasing away from it. This ensures convergence of the integral and justifies the saddle point approximation.

4.3 Neumann or Dirichlet boundary conditions?

Now that we have seen how the Picard-Lefschetz method enables one to compute a highly oscillating integral in principle, we can turn to explicit examples by considering once again the pure gravity case in minisuperspace. The trick is to use the metric

$$\mathrm{d}s^2 = -\frac{N^2}{q(t)}\mathrm{d}t^2 + q(t)\mathrm{d}\Omega_3^2 \,, \tag{94}$$

because in these variables, the path integrals on q and its momentum become Gaussian integrals.

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With this new metric, the (Lorentzian) Einstein-Hilbert action of a closed space ($k = 1$) and its equations of motion read:

$$\begin{aligned} S_{\text{E-H}} &= \frac{1}{2}\int_{\mathcal{M}} \mathrm{d}^4x\sqrt{-g}(R-2\Lambda) + \int_{\partial\mathcal{M}_{\mathrm{f}}} \mathrm{d}^3y\,\sqrt{h}K\,, \\ &= 2\pi^2\int_0^1 \mathrm{d}t\left[\frac{-3\dot{q}^2}{4N} + N(3-\Lambda q)\right] - 2\pi^2\left[\frac{3q\dot{q}}{2N}\right]^0, \end{aligned} \quad \Rightarrow \quad \begin{cases} \ddot{q} = \dfrac{2\Lambda}{3}N^2\,; \\ \dfrac{\dot{q}^2}{4N^2} + 1 = \dfrac{\Lambda}{3}q\,. \end{cases} \tag{95}$$

The classical solution with fixed Dirichlet boundary conditions $q(t=0) = 0$ and $q(t=1) = q_1$ is then

$$\bar{q}(t) = \frac{\Lambda N^2}{3}t(t-1) + q_1 t\,. \tag{96}$$

Therefore, the full solution $q(t)$ is given by this classical solution $\bar{q}(t)$, plus some arbitrary fluctuation $Q(t)$ satisfying the boundary conditions: $q(t) = \bar{q}(t) + Q(t)$.

The boundary conditions that one imposes at $t = 0, 1$ must be consistent with the variational principle. Since for the no-boundary condition we added a GHY term on the final boundary $t = 1$ but not at the origin $t = 0$, the requirements will be different. We calculate

$$\delta_q S_{\text{E-H}} = 2\pi^2\int_0^1 \mathrm{d}t\left[-\frac{6\dot{q}\,\delta\dot{q}}{4N} - N\Lambda\delta q\right] - 2\pi^2\left[\frac{3\delta q\,\dot{q}}{2N} + \frac{3q\,\delta\dot{q}}{2N}\right]^0 \tag{97}$$

$$= 2\pi^2\int_0^1 \mathrm{d}t\left[\frac{3\ddot{q}}{2N}\delta q - N\Lambda\delta q\right] - 2\pi^2\left[\frac{3\dot{q}\,\delta q}{2N}\right]^1 - 2\pi^2\left[\frac{3q\,\delta\dot{q}}{2N}\right]^0. \tag{98}$$

On the final hypersurface boundary in $t = 1$, we must have $\left.\dfrac{3\dot{q}\delta q}{2N}\right|_1 = 0$, therefore we can impose Dirichlet boundary conditions: $q(1) = q_1, Q(1) = 0$.

On the initial hypersurface boundary, we need to have $\left.\dfrac{3q\delta\dot{q}}{2N}\right|_0 = 0$, so we have two possible choices. The first is to set as boundary condition $q|_0 = 0$, i.e., $\bar{q}|_0 = 0$ and $Q|_0 = 0$: this leads to the Dirichlet-Dirichlet no-boundary proposal. The second choice is to impose a boundary condition on the momentum of the scale factor initially, $\dot{Q}|_0 = 0$. This is what we call the Neumann-Dirichlet no-boundary proposal. We now consider these two possibilities.

Dirichlet initial boundary conditions The most natural choice which follows the philosophy of the no-boundary proposal is to choose Dirichlet boundary conditions at both ends: $Q(0) = Q(1) = 0$. This Dirichlet-Dirichlet boundary condition implies that the path integral is summing only over compact metrics.

Note that in these lectures we are only considering the case where $q_1 > 3/\Lambda$. The case $q_1 < 3/\Lambda$ can also be studied and yields a different structure for the thimbles and saddle point locations [47].

Thanks to the form of the metric (94), the path integral over the scale factor becomes a Gaussian

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integral that can be evaluated exactly:

$$\Psi_{\mathrm{DD}}[0,q_1] = \int_0^\infty \mathrm{d}N \exp\left[\frac{i}{\hbar}S_{\text{E-H}}[\bar{q}(t)]\right]\int_{Q(0)=0}^{Q(1)=1}\mathcal{D}Q\exp\left[-\frac{2\pi^2 i}{\hbar}\int_0^1 \mathrm{d}t\frac{3\dot{Q}^2}{4N}\right] \tag{99}$$

$$= \int_0^\infty \mathrm{d}N\sqrt{\frac{3\pi i}{2N\hbar}}\exp\left[\frac{i}{\hbar}S_{\text{E-H}}[\bar{q}(t)]\right], \tag{100}$$

$$= \int_0^\infty \mathrm{d}N\sqrt{\frac{3\pi i}{2N\hbar}}\exp\left[\frac{2\pi^2 i}{\hbar}\left(\frac{\Lambda^2N^3}{36}+N\left(3-\frac{\Lambda q_1}{2}\right)-\frac{3q_1^2}{4N}\right)\right]. \tag{101}$$

Now in order to evaluate the lapse integral, we apply the Picard-Lefschetz method. We first calculate the saddle points:

$$\left.\frac{\partial S_{\text{E-H}}[\bar{q}(t)]}{\partial N}\right|_{N_\sigma} = 0 \;\Leftrightarrow\; \frac{\Lambda^2N_\sigma^2}{12}+\left(3-\frac{\Lambda q_1}{2}\right)+\frac{3q_1^2}{4N_\sigma^2} = 0\,, \tag{102}$$

$$\Leftrightarrow \quad N_\sigma^{2\,(\pm)} = \frac{9}{\Lambda^2}\left[\frac{\Lambda q_1}{3}-2\pm 2i\sqrt{\Lambda q_1 - 3}\right] \quad\Leftrightarrow\quad N_\sigma^{(\pm\pm)} = \pm\frac{3}{\Lambda}\left[\sqrt{\frac{\Lambda q_1}{3}-1}\pm i\right]. \tag{103}$$

We find four saddle points (corresponding to the two Vilenkin ($\mathrm{Im}[N_\sigma] > 0$) and two Hartle-Hawking ($\mathrm{Im}[N_\sigma] < 0$) one, as in figure 5). They are plotted on the left panel of figure 7 for $q_1 = 10H^{-2}$, together with the steepest descent and ascent lines found by the contour plot of $\mathrm{Re}(S[N]) = \mathrm{Re}(S[N_\sigma])$, while the density plot of $-\mathrm{Im}(S[N])$ shows the regions of convergence (in blue) and divergence (in red) of the integral.

If the integral contour initially runs along the real semi-axis $N \in (0,+\infty)$, then we find that it is deformed through the vertical steepest ascent line into the steepest descent line in the upper-right quadrant, hence selecting one Vilenkin saddle point. In fact, whatever the original line of integration is, we find that the Vilenkin saddle points will always be selected[18]. This means that when applying the natural definition of the no-boundary proposal in the Lorentzian path integral formulation, we actually end up with the Vilenkin wavefunction.

If we are starting from the semi-real axis $N \in (0,+\infty)$, then the only saddle that is picked by the Picard-Lefschetz theory is the one in the upper-right quadrant, $N_\sigma^{(++)}$. Then the path integral becomes:

$$\Psi_{\mathrm{DD}}[0,q_1] = \sqrt{\frac{3\pi i}{2\hbar}}\int_{\mathcal{J}_{(++)}}\mathrm{d}N\,\frac{e^{2\pi^2 i f_0(N)/\hbar}}{\sqrt{N}}\,, \tag{104}$$

where $f_0(N) = \dfrac{\Lambda^2N^3}{36}+N\left(3-\dfrac{\Lambda q_1}{2}\right)-\dfrac{3q_1^2}{4N}$. We can then Taylor-expand around the saddle point

[18] In fact, we are here in presence of a Stokes phenomenon, so we should first deform the action by an infinitesimal amount (in the parameter $\hbar$ for instance). Recently it has been shown that the ambiguity coming from the Stokes phenomenon cancels another ambiguity coming from applying resurgence in order to calculate the integral over the weighting (90) exactly [21].

PoS(Modave2024)003

$N_\sigma^{(++)}$ to obtain:

$$\Psi_{\rm DD}[0,q_1] \simeq \sqrt{\frac{3\pi i}{2\hbar}} \frac{e^{2\pi^2 i f_0(N_\sigma^{(++)})/\hbar}}{\sqrt{N_\sigma^{(++)}}} \int_{\mathcal{J}_{(++)}} \mathrm{d}N\, e^{\frac{\pi^2 i}{\hbar}\frac{\partial^2 f_0}{\partial N^2}\cdot\left(N-N_\sigma^{(++)}\right)^2} \left(1+O(\hbar^{1/2})\right), \tag{105}$$

$$\simeq \sqrt{\frac{3\pi i}{2\hbar}} \frac{e^{2\pi^2 i f_0(N_\sigma^{(++)})/\hbar}}{\sqrt{N_\sigma^{(++)}}} e^{i\theta_\sigma} \int_0^{+\infty} \mathrm{d}n\, e^{-\frac{\pi^2}{\hbar}\left|\frac{\partial^2 f_0}{\partial N^2}\right| n^2} \left(1+O(\hbar^{1/2})\right)\,; \tag{106}$$

$$\Psi_{\rm DD}(q_1) \simeq \sqrt{\frac{3\pi i}{2N_\sigma \hbar}} \exp\left[\frac{2\pi^2 i}{\hbar}\left(\frac{\Lambda^2 N_\sigma^{(++)\,3}}{36} + N_\sigma^{(++)}(3-\Lambda q_1/2) - \frac{3q_1^2}{4N_\sigma^{(++)}}\right)\right], \tag{107}$$

$$= \sqrt{\frac{3\pi(1+i\sqrt{\Lambda q_1/3-1})}{2\hbar q_1}} \exp\left[-\frac{12\pi^2}{\hbar\Lambda} - \frac{12\pi^2 i}{\hbar\Lambda}\sqrt{\Lambda q_1/3-1}\right]. \tag{108}$$

The problem here is that the Vilenkin saddle points are actually unstable against the addition of perturbations. In particular, one finds that anisotropic configurations have a higher weigthing than isotropic ones, leading to a non-normalisable and ill-defined wavefunction [45].

Neumann initial boundary conditions A possible solution, although one could argue that its interpretation would deviate from the original no-boundary idea, is to sum rather on regular metrics, i.e., metrics starting with an initial zero momentum flow [48]. This means that the boundary conditions are Neumann-Dirichlet boundary conditions: $\dot q(0) = 2Ni\,,\ q(1) = q_1\,,$ so the classical solution transforms into

$$\bar q_{\rm N}(t) = \frac{\Lambda N^2}{3}(t^2-1) + 2Ni(t-1) + q_1\,. \tag{109}$$

The scale factor integral over fluctuations also changes (see the Appendix of [49] for an explicit calculation) and we find:

$$\Psi_{\rm ND}[q_1] = \int_0^\infty \mathrm{d}N \exp\left[\frac{i}{\hbar}S_{\text{E-H}}[\bar q_{\rm N}(t)]\right] \int_{\dot Q(0)=0}^{Q(1)=0} \mathcal{D}Q \exp\left[-\frac{2\pi^2 i}{\hbar}\int_0^1 \mathrm{d}t \frac{3\dot Q^2}{4N}\right], \tag{110}$$

$$= \int_0^\infty \mathrm{d}N \sqrt{\frac{3\pi i}{\hbar}} \exp\left[\frac{i}{\hbar}S_{\text{E-H}}[\bar q_{\rm N}(t)]\right], \tag{111}$$

$$= \int_0^\infty \mathrm{d}N \sqrt{\frac{3\pi i}{\hbar}} \exp\left[\frac{2\pi^2 i}{\hbar}\left(\frac{\Lambda^2 N^3}{9} + \Lambda N^2 i - N\Lambda q_1 - 3iq_1\right)\right]. \tag{112}$$

The saddle points are found through:

$$\left.\frac{\partial S_{\text{E-H}}[\bar q_{\rm N}(t)]}{\partial N}\right|_{N_\sigma} = 0 \;\Leftrightarrow\; \frac{\Lambda^2 N_\sigma^2}{3} + 2\Lambda N_\sigma i - \Lambda q_1 = 0\,, \tag{113}$$

$$\Leftrightarrow\quad N_\sigma^{(\pm)} = -\frac{3}{\Lambda}\left[i \pm \sqrt{\Lambda q_1/3-1}\right]. \tag{114}$$

With Neumann-Dirichlet boundary conditions, we therefore only obtain two saddle points. These are the Hartle-Hawking saddle points ($\mathrm{Im}(N_\sigma) < 0$). This is due to the fact that we have already

PoS(Modave2024)003

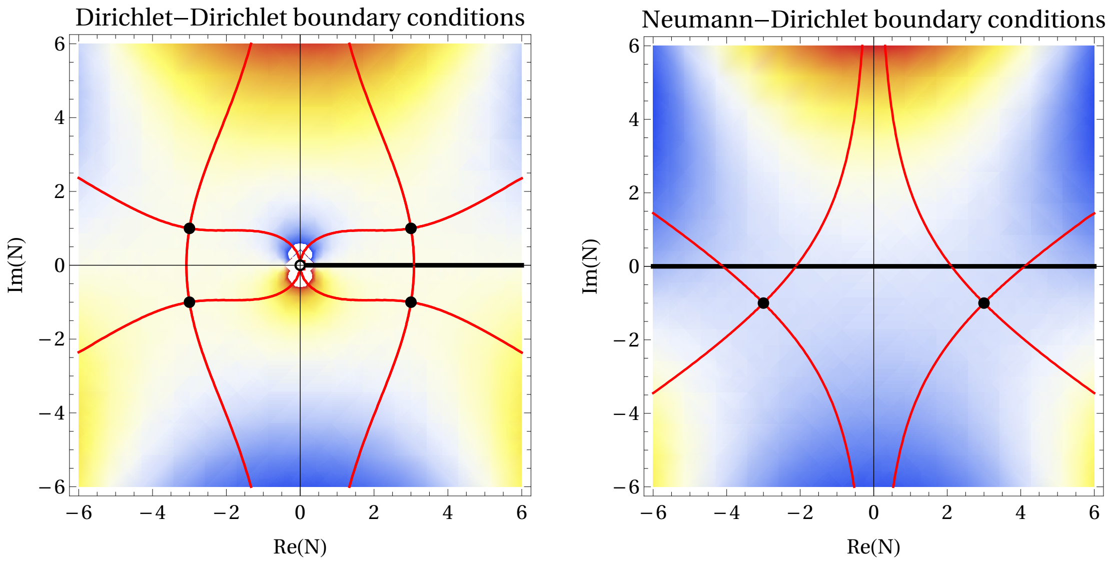

Figure 7: Regions of convergence/divergence of the path integral (the integrand tends to converge (diverge) the bluer (the redder)), steepest ascent and descent paths in red solid lines, and saddle points as black dots for the no-boundary solutions with Dirichlet boundary conditions (**sum over compact metrics**, with $q(0) = 0$ and $q(1) = 10H^{-2}$) on the left, and for Neumann boundary conditions (**sum over regular metrics**, with $q(1) = 10\,H^{-2}$) on the right. On the left, the real axis can be deformed following the steepest ascent into the steepest descent lines intersecting it at the saddle points in the upper half plane. These upper saddle points are unstable and correspond to the Vilenkin wavefunction. On the right, the sum over regular metrics automatically restricts to the stable lower saddle points that are then selected by the Picard-Lefschetz theory and yields the Hartle-Hawking wavefunction.

fixed the sign in the initial momentum, i.e., we have effectively already chosen one direction for the Wick rotation. The Picard-Lefschetz theory applied in this case automatically selects the stable, Hartle-Hawking saddle points (see right panel of figure 7), and we recover the Hartle-Hawking wavefunction:

$$\begin{aligned}
\Psi_{\rm ND}[q_1] &\simeq \sqrt{\frac{3\pi i}{\hbar}}\left[e^{\frac{2\pi^2 i}{\hbar}\left(\frac{\Lambda^2 N^{(+)3}}{9}+\Lambda N^{(+)2} i - N^{(+)}\Lambda q_1 - 3 i q_1\right)} + e^{\frac{2\pi^2 i}{\hbar}\left(\frac{\Lambda^2 N^{(-)3}}{9}+\Lambda N^{(-)2} i - N^{(-)}\Lambda q_1 - 3 i q_1\right)}\right] \\
&\simeq \sqrt{\frac{3\pi i}{\hbar}}\exp\left[\frac{12\pi^2}{\Lambda\hbar}\right]\cdot 2\cos\left(\frac{12\pi^2}{\Lambda\hbar}\sqrt{\Lambda q_1/3-1}^{\,3}\right). \qquad (115)
\end{aligned}$$

With this method we can only obtain the approximate solution at the lowest order in $\hbar$. However, it has been shown recently that one can use resurgence to resum the series exactly, and recover the Airy functions for both the Dirichlet-Dirichlet and the Neumann-Dirichlet case [21].

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