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TESE DE CONCLUSÃO DE DOUTORADO EM FÍSICA

Gravitational Particle Creation in Bouncing Cosmological Models

Diogo C. F. Celani

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Nelson PINTO-NETO

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Abstract

In this thesis, we calculate gravitational scalar particle creation in quantum cosmological bouncing models derived from the de Broglie–Bohm interpretation of quantum mechanics applied to the Wheeler–DeWitt equation in minisuperspace. We consider the scalar field either conformally or minimally coupled to gravity, and it may be massive or massless, without self interaction. The generalization to any other constant value of the gravitational coupling is simple enough. We consider particle creation in two bouncing models: the first is a single fluid model dominated by radiation; the second, more realistic model is composed of dust and radiation such that radiation dominates near the bounce, while the dust fluid only dominates far from the bounce. The conformally coupled case is a useful prototype to investigate the minimally coupled case because the asymptotic solutions to the Klein–Gordon equation do not depend on the gravitational coupling. Moreover, in the pure radiation model, the solutions with conformal coupling are exact. However, particle creation with conformal coupling is negligible in both models. In the case of massive minimally coupled particles, we find the same results in both models within observational constraints: particle number is most important at the bounce energy scale, and it is not sensitive neither to its mass nor whether there is dust in the background model. This conclusion, however, may change for supermassive particles with masses near or larger than the bounce energy scale, which we did not consider. Nevertheless, the energy density of the massive particles do depend on their masses and on the energy scale of the bounce. For very large masses and deep bounces, this density may even overcome that of the background. In the case of massless minimally coupled particles, the energy density may become comparable to that of the background only for extreme bounces at energy scales close to the Planck scale, which lies beyond the scope of our calculations: the Wheeler–DeWitt approach we take is expected to break near such high energy regime. Finally, in the model with dust and radiation, there is an infrared divergence for massless minimally coupled particles, which becomes important only for scales much larger than the present Hubble radius.

Resumo

Nesta tese, calculamos a criação gravitacional de partículas escalares em modelos cosmológicos com ricochete derivados da equação de Wheeler–DeWitt na interpretação de Broglie–Bohm da mecânica quântica. Consideramos que o campo escalar está conformemente ou minimamente acoplado à gravidade e pode ser massivo ou sem massa, sem auto–interação. A generalização para qualquer outro valor constante do acoplamento gravitacional é imediata. Consideramos a criação de partículas em dois modelos: o primeiro é um modelo com um fluido de radiação apenas; o segundo modelo, mais realista, é composto por poeira e radiação, de modo que a radiação domina no ricochete, enquanto a poeira domina apenas assintoticamente. O caso conforme é um protótipo útil para investigar o caso minimamente acoplado, uma vez que as soluções assintóticas da equação de Klein–Gordon não dependem do acoplamento gravitacional. Além disso, no modelo apenas com radiação, as soluções com acoplamento conforme são exatas. Contudo, a criação de partículas com acoplamento conforme é desprezível em ambos os modelos. No caso de partículas massivas minimamente acopladas, para valores dos parâmetros de acordo com os vínculos observacionais, encontramos os mesmos resultados em ambos os modelos: o número de partículas criadas é mais importante na escala de energia do ricochete, e não é sensível nem à massa, nem a presença de poeira no modelo. Contudo, esta conclusão não inclui partículas supermassivas com massas próximas ou maiores que a escala de energia do bounce, caso que não consideramos. No entanto, a densidade de energia das partículas massivas depende das suas massas e da escala de energia do ricochete. Para massas muito grandes e ricochetes profundos, a densidade de energia das partículas criadas pode até superar a densidade do background. No caso de partículas minimamente acopladas sem massa, a densidade de energia pode tornar-se comparável à do background apenas para ricochetes extremos em escalas de energia próximas à escala de Planck, que está além do limite de validade de nossos cálculos: a equação de Wheeler–DeWitt que usamos não deve ser válida em um regime de energia tão extremo. Finalmente, no modelo com poeira e radiação, existe uma divergência infravermelha para partículas minimamente acopladas sem massa, que só se torna importante para escalas muito maiores do que o atual raio de Hubble.

To my family.

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Even though my mother was a math teacher, the love for knowledge and books I inherited from my father. I read many of his books, and not surprisingly it was science fiction that caught most of my attention. Man, I loved those Perry Rhodan books! Although I miss him, I am grateful for the time we had together. Those good memories and his example helped shaping me.

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Notation

Here we collect some of the notation used throughout the text. They are also explained within the text. Throughout this work we use the metric with signature $(+, -, -, -)$, except in the section on the Hamiltonian of general relativity.

\dot{a} denotes the derivative with respect to cosmic time.

a' denotes the derivative with respect to conformal time.

L_b is curvature scale at the bounce.

$L_c = 1/m$ is the Compton wavelength of a particle with mass m .

$r_b = L_b/L_c$.

a_0 is the present value of the scale factor and H_0 the present Hubble rate.

a_b is the scale factor at the bounce.

a_e is the scale factor at radiation–matter equality.

$x = a_0/a$ is a redshift–like parameter.

It may be that save in this little planet, this speck of cosmic dust, invisible long before the nearest star could be attained — it may be, I say, that nowhere else does this thing called pain occur.

The Island of Dr. Moreau, H. G. Wells

Were this world an endless plain, and by sailing eastward we could for ever reach new distances, and discover sights more sweet and strange than any Cyclades or Islands of King Solomon, then there were promise in the voyage. But in pursuit of those far mysteries we dream of, or in tormented chase of the demon phantom that, some time or other, swims before all human hearts; while chasing such over this round globe, they either lead us on in barren mazes or midway leave uswhelmed.

Moby Dick, Herman Melville

A vida é resolver equações diferenciais.

Sandro Vitenti

Chapter 1

Introduction

In order to seek truth, it is necessary once in the course of our life to doubt, as far as possible, of all things.

René Descartes

The persistence of long-standing issues in the scenario of cosmic inflation, the leading framework to explain the initial conditions for the standard Big Bang model of cosmology, motivates the search for alternatives. One such alternative that has been gaining attention is the paradigm of bouncing cosmology [1–3]. In this scenario, the universe contracts from a very large size and, as it becomes sufficiently small, some exotic material or quantum gravity effects take place and make the universe bounce, thereby expanding into the standard model afterwards. In this case, the initial singularity present in the standard model is solved by construction. Moreover, the bouncing scenario can also solve other puzzles of the standard cosmology (as the horizon and flatness problems) and provide a causal mechanism to generate primordial cosmological perturbations from quantum vacuum fluctuations, with an almost scale invariant spectrum, just like inflation does but from a different perspective. The bouncing scenario may therefore be viewed as a realistic alternative to inflation, although they do not necessarily exclude each other.¹

There are many known mechanisms that can generate a bounce, and there are also many open questions and issues to be investigated concerning these models, for general reviews see [1,3]. Sadly, but also understandably, most studies on such alternative models are restricted to cosmological perturbation theory and to the question whether these models can generate an almost scale invariant spectrum that could have given birth to the

¹However, we only consider the observationally interesting cases where the bouncing effects are not diluted by inflation.

present large scale structure of the universe through gravitational instability. This is simply because there lies the greatest possibility to make contact with observations. However, other important physical mechanisms such as particle creation, baryogenesis, and others remain largely unexplored in those scenarios. It is interesting though that much of the research on these processes already done in the inflationary scenario may be adapted to alternative scenarios, or at least be useful as a starting point.

In this thesis we are concerned with gravitational particle creation by the bouncing background dynamics. Is it large enough to modify the background and even prevent the bounce causing a collapse? Can it induce some sort of reheating, making the model asymmetric around the bounce? Or is it always negligible? The aim of this thesis is thus to calculate gravitational particle creation in bouncing models. In the models considered, the bounce is due to quantum cosmological effects when the curvature of space–time becomes very large: the models are derived from the de Broglie–Bohm interpretation of quantum mechanics applied to the Wheeler–DeWitt equation restricted to minisuperspace (the usual Copenhagen point of view cannot be used in quantum cosmology, see [2] and references therein for a review on this subject). The Bohmian trajectories describing the scale factor evolution are calculated and they are non–singular, presenting a bounce due to quantum effects at small scales, and turning to a classical standard evolution when the scale factor becomes sufficiently large. These models contain one single hydrodynamical fluid, or two: the usual observed radiation and dust contents which are present in our universe. Note that apart from the use of the de Broglie–Bohm interpretation of quantum mechanics, these models are conservative in that the Hamiltonian of general relativity is quantized and there is only radiation and dust in the background, with no exotic fluids violating the energy conditions.² We expect that the simple Wheeler–DeWitt approach we are using should be valid only at scales some few orders of magnitude below the Planck energy, being a limit of some more fundamental theory of quantum gravity suitable for energy scales close to or above the Planck scale.

In chapter 2, we present a brief review on classical cosmology. We introduce the standard big bang model in section 2.1. In section 2.2, we introduce the paradigm of inflation. In section 2.3, we try to motivate the idea of a bouncing universe. In chapter 3, we derive the two models we use to calculate particle creation. In section 3.1, we briefly introduce the Hamiltonian approach to general relativity. In section 3.2, we explain why the Copenhagen interpretation of quantum mechanics, usually taught in classes and in text–books, is not suitable to quantum cosmology. In section 3.3, we give a sketchy derivation of the models we use to calculate the Bogoliubov coefficients. These first two chapters are completely review with nothing whatsoever original. In chapter 4, we finally arrive at the results. In sections 4.1 and 4.2, we give a very brief review on quantization of scalar fields in curved space. After that, we are finally in place to calculate the Bogoliubov coefficients in section 4.3. Note that this thesis is very interdisciplinary and there are whole books dedicated to most of the

²Although, in practice, the models can be effectively described as if there is stiff matter with negative energy density dominating near bounce.

sections. That is why this thesis is necessarily incomplete or not self-contained. A note on the bibliography. I have made no attempt to make references to the original literature. Instead, the selection of the works, where the original literature can be found, come from my own biased point of view. Finally, our results can also be found in [4].

Chapter 2

Standard Cosmology, Inflation, and the Bouncing Universe

Few if any seemed to have grasped the truest principle of reality: new knowledge leads to yet more awesome mysteries.

Stephen King, *The Gunslinger*.

In this chapter, we outline the basic cosmological theory that is relevant to our work. In section 2.1, we briefly introduce the standard big bang model [5–13], which is based on two well-tested pillars of physics, general relativity and nuclear physics. It explains the origin of the cosmic microwave background radiation (CMBR) and it accounts for the abundances of light elements through the process of primordial nucleosynthesis. However, the picture is clearly incomplete for some reasons that are mainly theoretical in nature; a fact that calls for speculations on the physics of the early universe.

At present, the leading working hypothesis to explain the initial conditions for the standard model is the paradigm of cosmic inflation [14–19], which is the subject of the section 2.2. In that picture, the universe underwent an early period of nearly exponential growth driven by a scalar field that dominated at that time. In that way, inflation is intended to solve the classic puzzles of the standard model and to account for the observed temperature perturbations in the CMBR that gave rise to the present large-scale structure of the universe through gravitational instability.

Finally, in the section 2.3, we try to motivate the idea of a bouncing cosmology [1–3, 20–22]. Unlike the standard model and the inflationary paradigm, the bouncing universe is singularity-free by construction and it can

also solve the classic puzzles [20]. Moreover, it can produce an almost scale invariant spectrum of perturbations. However, tensor perturbations in these models are generally very tiny and undetectable: if primordial gravitational waves are confirmed, many bouncing models would be in trouble [3]. Like inflation or any other paradigm of the early universe, the bouncing paradigm has its own problems, which deserve further investigation.

It should be noted that everything in this chapter has the character of a review, that is, nothing here is original. Also, I will mainly quote the cosmological parameters from [23], but one should keep in mind that the precision of observations is constantly increasing, and that these values (with their errors) do slightly depend on the experiment so that they may be taken in a qualitative fashion. As a final note, I mention that the inflationary paradigm is so successful that it is indeed included in the "standard model", however, only for the sake of presentation I keep it separated.

2.1 Standard Model

There are many excellent books on cosmology [5–13]. Interesting accounts on conceptually related issues include [24–26]. The standard model of cosmology accurately describes the history of the universe since the radiation-dominated phase some 13.8 billion years ago [23].

The starting point is the assumption of the cosmological principle.¹ It states that the distribution of matter in the universe can be described as approximately homogeneous and isotropic when averaged at large enough spatial scales, ~ 100 Mpc. This is important because these symmetries [28] result in simplifications in the Einstein equations, which allow to describe the universe with simple mathematical models. The cosmological principle is supported by several observations, in particular the CMBR and deep galaxy surveys.

Another pillar of the standard model was the discovery by Edwin Hubble that the universe is actually expanding. At that time, around the 1920s, the universe was believed to be static. His discovery followed from observations of redshifts of nearby galaxies. He also found a linear correlation between the distances and velocities of galaxies. There are now several independent observations that support the expansion of the universe. In the light of general relativity, the expansion means that space is stretching itself with the result that the physical distance between co-moving galaxies is increasing. Hubble’s discovery (together with the realization that the nebulae are actually galaxies outside the Milk Way) marks the beginning of modern cosmology.

The current expansion also means that the universe was smaller in the past, and therefore denser and also hotter. In fact, so dense and hot that the short-range nuclear interactions were more effective than the gravitational expansion. The creation of the first atoms can be accurately described from basic principles of nuclear physics and thermodynamics. This process is called primordial nucleosynthesis. It accounts for the abundances of the light elements (the ones not formed in the interiors of stars or supernovae) with the possible exception of the lithium problem [29], and it also explains the origin of the CMBR.

2.1.1 Friedmann Expansion

In general relativity, as in any geometric theory of gravity,² the cosmological principle implies that the background metric of the universe can be approximately described by a very simple geometry with only one unknown function of time. The metric written in coordinates such that the symmetries of the cosmological

¹An interesting historical account of the cosmological principle up to the end of the 1970s can be found in [27] and references therein. Moreover, Weinberg cites some alternative views in [10].

²The FLRW metric can be deduced based on purely geometric reasoning, without any reference to the Einstein equations.

principle are explicit is called the Friedmann-Lemaître-Robertson-Walker metric [9, 28]

$$ds^2 = dt^2 - a^2(t) \left[\frac{dr^2}{1 - \mathcal{K}r^2} + r^2 (d\theta^2 + \sin^2\theta d\phi^2) \right] \quad (2.1)$$

where r , θ and ϕ are the comoving coordinates and t is the cosmic time [28]; the scale factor $a(t)$ describes the stretching (or contraction) of physical space over time; $\mathcal{K} = 0, \pm 1$ represents the constant curvature of the spatial sections. Sometimes, it is also convenient to use the conformal time η defined as

$$d\eta = \frac{dt}{a(t)} \quad (2.2)$$

which may simplify some equations. The expansion (contraction) of the universe is determined by the Hubble rate,

$$H = \frac{\dot{a}}{a}, \quad (2.3)$$

which also furnishes a relevant time scale. It also links the radial speed of a galaxy to its distance through the Hubble law, $v = Hd$, which is the only expansion law consistent with the cosmological principle. The present value of the Hubble rate is $H_0 = 100 h \text{ km sec}^{-1} \text{ Mpc}^{-1} = 2 h \times 10^{42} \text{ GeV}$, where $h = 0.67$ [23] contains the uncertainty on the value of H_0 .

Assuming a perfect fluid description for the matter in the universe, with energy density ρ and pressure p , the cosmological principle also restricts the shape of the energy-momentum tensor which implies that the Einstein equations reduce to the Friedmann equations

$$H^2 = \frac{8\pi G}{3}\rho - \frac{\mathcal{K}}{a^2} + \frac{\Lambda}{3} \quad (2.4)$$

$$\frac{\ddot{a}}{a} = -\frac{4\pi G}{3}(\rho + 3p) + \frac{\Lambda}{3} \quad (2.5)$$

The stress-energy conservation equation, $T_{;\nu}^{\mu\nu} = 0$, reduces to a single equation

$$\dot{\rho} + 3H(\rho + p) = 0, \quad (2.6)$$

but this equation is not independent of the Friedmann equations [9]. These equations need to be supplemented by one more equation that relates ρ and p , which is called the equation of state,

$$p = \omega\rho. \quad (2.7)$$

Note that this equation is always true: whatever is the relation between density and pressure, one can always define ω so that (2.7) is satisfied. However, even in the simple cases where ω is constant there is some interesting

physics. A few examples are shown bellow.

Non-Relativistic Matter or Dust (with $\mathcal{K} = 0$ and $\Lambda = 0$)

The simplest case is that of dust, which can be described as a pressureless fluid, so that $\omega = 0 \rightarrow p = 0$. Equation (2.6) implies that

$$\rho \sim \frac{1}{a^3}, \quad (2.8)$$

as expected. Also, using (2.8) in (2.4),

$$a(t) \sim t^{2/3} \sim \eta^2. \quad (2.9)$$

Relativistic Matter or Radiation (with $\mathcal{K} = 0$ and $\Lambda = 0$)

In that case, $\omega = 1/3$ so that $p = \rho/3$. Equation (2.6) implies that

$$\rho \sim \frac{1}{a^4}, \quad (2.10)$$

so that the density of radiation is not only affected by the stretching of space, but also by the redshift of the wavelentghs. Again, using (2.10) in (2.4),

$$a(t) \sim t^{1/2} \sim \eta, \quad (2.11)$$

so that the pressure of radiation somewhat slows expansion or contraction. Similarly, radiation pressure also works against gravitational instability [9].

Stiff Matter (with $\mathcal{K} = 0$ and $\Lambda = 0$)

This is a more exotic example where the speed of sound equals the speed of light. This is sometimes postulated to be the effective behavior of matter at extremely high densities [30]. In that case, $\omega = 1$ so that $p = \rho$. Equation (2.6) implies that

$$\rho \sim \frac{1}{a^6}, \quad (2.12)$$

Again, using (2.12) in (2.4),

$$a(t) \sim t^{1/3} \sim \eta^{1/2}. \quad (2.13)$$

Constant Density (with $\mathcal{K} = 0$)

Another interesting case is the one for which $\omega = -1$. Equation (2.6) implies that

$$\rho \sim \text{const}, \quad (2.14)$$

so that the energy density is constant in time as in space. Note that Λ may be included in that energy density. Again, using (2.14) in (2.4)

$$a(t) \sim \exp\{Ht\} \sim -\frac{1}{H\eta}, \quad (2.15)$$

where H is constant and $\eta < 0$. An exponential expansion may have interesting consequences for early universe cosmology.

Constant Equation of State (with $\mathcal{K} = 0$ and $\Lambda = 0$)

Finally, for any constant equation of state, equation (2.6) implies that

$$\rho \sim a^{-3(1+\omega)}, \quad (2.16)$$

and (2.4) implies (as long as $\omega \neq -1$)

$$a(t) \sim a^{\frac{2}{3(1+\omega)}}, \quad (2.17)$$

which can be seen to agree with (2.9), (2.11) and (2.13) with the corresponding values of ω .

2.1.2 Density Parameters

It is useful to write the Friedmann equation in terms of dimensionless parameters so that different cosmological models can be compared according to their density parameters. The critical density ρ_c is defined as the energy density necessary to make the universe spatially flat. From the Friedmann equation (2.4), the critical density reads

$$\rho_c = \frac{3H^2}{8\pi G}. \quad (2.18)$$

The present critical density is

$$\rho_{c0} = \frac{3H_0^2}{8\pi G} = 1.88 h^2 \times 10^{-29} \text{g cm}^{-3}, \quad (2.19)$$

where, again, $h = 0.67$ [23]. Observations show that the present universe density is actually very close to the present critical density. The density parameters are defined as

$$\Omega = \frac{\rho}{\rho_c} = \frac{8\pi G}{3H^2}\rho. \quad (2.20)$$

They are therefore the ratios of the different contributions to the total energy density of the universe. The Friedmann equation (2.4) can thus be written as

$$\Omega_{m0} \left(\frac{a_0}{a}\right)^3 + \Omega_{\gamma 0} \left(\frac{a_0}{a}\right)^4 + \Omega_{s0} \left(\frac{a_0}{a}\right)^6 + \Omega_{\mathcal{K}0} \left(\frac{a_0}{a}\right)^2 + \Omega_{\Lambda} = 1, \quad (2.21)$$

where the subscripts m , γ , s , \mathcal{K} and Λ denote the different contributions from non-relativistic matter, radiation, stiff matter, curvature and dark energy (briefly explained below), respectively; moreover, $\Omega_{\mathcal{K}0} = -\mathcal{K}/a_0^2 H_0^2$ and $\Omega_{\Lambda} = \Lambda/3$.

According to cosmological observations, the contribution of baryons (protons, nuclei) into the total present energy density is only about $\Omega_{b0} \approx 0.049$ [23]; while the contribution from radiation is even smaller $\Omega_{\gamma 0} \approx 9.2 \times 10^{-5}$.³ The largest fraction of the total energy density in our universe is therefore unknown.

The dominant contribution of bound astronomical systems like galaxies or clusters, detectable only by its gravitational influence, is called dark matter [31]. There is convincing astronomical evidence (rotation curves of galaxies, dynamical stability of galaxies) that show that there is more clustering matter than one can see and cosmological evidence (primordial nucleosynthesis, CMBR anisotropy, cosmic structure formation) that show that dark matter cannot consist of known particles in the standard model of particle physics [12]. The present mass density of baryons and dark matter together is $\Omega_{m0} \approx 0.31$ [23].

The other unknown material is even more mysterious than dark matter. It is called dark energy and it is believed to drive the current accelerated expansion of the universe. This is not matter consisting of unknown particles, but some vacuum-like kind of energy. It does not aggregate into clusters like ordinary matter and, therefore, its effects are only observed at cosmological scales. An important property of dark energy is that as the universe expands, its density either depends on time very weakly or does not depend on time at all. Hence, as the energy density of radiation and matter fall with a^{-4} and a^{-3} , respectively, dark energy starts to dominate at some stage of the cosmological evolution. The transition from dust-dominated to dark energy dominated expansion occurred very recently in our universe at redshift $z \approx 0.29$.⁴ The age of the universe, structure formation, CMBR anisotropy all indicate that the present density of dark energy is $\Omega_{\Lambda} \approx 0.69$ [23].

³ $\Omega_{\gamma 0}$ can be calculated from Ω_{m0} and z_{eq} , the redshift at radiation-matter equality, as $\Omega_{\gamma 0} = \Omega_{m0}/(z_{eq} + 1)$ [9]. These can be found in table 4 in [23].

⁴Similarly to the calculation of the radiation density parameter, we can calculate this using $\Omega_{\Lambda} = \Omega_{m0}(z_{\Lambda} + 1)^3$ at equality [9].

2.1.3 Thermal History

From very basic principles, one can understand the behavior of matter at different stages in the history of the universe. Here, we are concerned with the beginning of the primordial nucleosynthesis which is one of the cornerstones of the standard model of cosmology. We then estimate a conservative lower bound on the energy scale (time scale) at which an early universe paradigm may have taken place. A more detailed account can be found, for instance, in [9].

Let Γ be the reaction rate for a given particle interaction. If that reaction rate is much higher than the expansion rate H , then the involved interaction can maintain those particles in a thermodynamic equilibrium at a temperature T : they can then be treated as Fermi-Dirac or Bose-Einstein gases, obeying their correspondent distribution functions. However, if $\Gamma < H$ the particle is said to be decoupled and evolves free of that reaction. Given that the temperature decays as the universe expands, there is always a temperature for which the interaction is not effective anymore; it is said to be "frozen".

At $T \sim 1$ MeV certain weak interaction processes fall out of equilibrium [9]. The primordial neutrinos decouple from the other particles and the ratio of neutrons to protons freezes out. The surviving neutrons determine the abundances of the primordial elements. At higher temperatures, photodissociation prevents any complex nuclei to form. This temperature therefore marks the beginning of primordial nucleosynthesis. At that time the universe was radiation-dominated with temperature described by the Stefan–Boltzmann law,

$$\rho \sim T^4, \tag{2.22}$$

which, together with equation (2.10), implies

$$a \sim \frac{1}{T}. \tag{2.23}$$

Assuming (correctly) that the universe was radiation-dominated for most of its expanding history, one can use the CMB temperature to estimate the scale factor at the beginning of primordial nucleosynthesis

$$x_n = \frac{a_0}{a_n} = \frac{T_n}{T_0} \approx \frac{10 \text{ MeV}}{2.7 \text{ K}} \approx 10^{11}. \tag{2.24}$$

Later, we will use this to restrict the scale factor at which a bouncing model may take place without spoiling the predictions of nucleosynthesis, $x_b > 10^{11}$. Note that we have used a conservative value of the temperature to calculate (2.24).

In passing, one may also estimate the scale factor at the Planck energy scale

$$x_p = \frac{a_0}{a_p} = \frac{T_p}{T_0} \approx \frac{1.2 \times 10^{19} \text{ Gev}}{2.7 \text{ K}} \approx 10^{31}, \quad (2.25)$$

which implies that in a semi-quantum bouncing model, $x_b < 10^{31}$.⁵ Putting (2.24) and (2.25) together, gives the allowable range

$$10^{11} < x_b < 10^{31}, \quad (2.26)$$

for the minimum scale factor at the bouncing phase.

⁵We use the unusual term "semi-quantum" instead of the commonly used "semi-classical" because the Bohmian trajectories for the scale factor are obtained in a quantum cosmological setting (more on this later).

2.2 Cosmic Inflation

The leading working hypothesis to explain the initial conditions for the standard big bang model is the paradigm of cosmic inflation [14–19]. According to inflation, the universe underwent a period of exponential growth driven by a scalar field that dominated the very early universe when it emerged from the quantum gravity era.⁶ It is claimed that inflation solves the classic puzzles of the standard big bang model [14] and accounts for the observed temperature perturbations in the CMBR that gave rise to the present large-scale structure of the universe through gravitational instability.

2.2.1 Puzzles in the Hot Big Bang Model

Although the standard big bang model can explain many observed features in the history of the universe, it presents some issues that cannot be explained within the model. These issues point to the inevitable conclusion that the standard model is incomplete. Some of these problems are listed below. Except for the singularity issue [33], inflation is usually claimed to solve these problems.

Singularity

The use of classical general relativity to describe the standard model of cosmology implies that there was in a finite past a gravitational singularity. This is a point (more precisely, a space-like surface) where no physics is possible [1, 25].

Horizon Problem

The distant regions of the universe, which could never have been in causal contact in the big bang model, seem to be at almost the same temperature. In other words, in the standard model there can be no causal mechanism that can explain why such remote regions have the same temperature.

⁶There are exceptions as described for instance in [32] where inflation is driven by gauge fields.

Flatness Problem

The observed flat geometry of the universe is unstable in a matter or radiation dominated phase, according to the Friedmann equations. The hot big bang model requires a fine-tuning of the density parameter in the past.

Exotic Relics Problem

As the universe cools down from the big bang, grand unified theories propose that the electro-weak and the strong forces arise due to spontaneous symmetry breaking from a single gauge theory. Such phase transition is model dependent but it generally predicts that heavy amounts of exotic relics are produced, which is in conflict with observations.

Structure Formation

The standard model cannot explain the observed large scale structure of the universe. If the perturbations are originated at the radiation dominated phase of the hot big bang model, then there has been no time for these perturbations to grow at the level observed today.

2.2.2 Inflationary Expansion

Consider a toy model with a single fluid. The second Friedmann equation (2.5) says that an accelerating universe requires

$$p < -\frac{\rho}{3}. \quad (2.27)$$

In the particular case that $p = -\rho$, equation (2.14) says that the density is constant and the expansion is exponential as in (2.15). Note that once exponential expansion begins, the curvature term \mathcal{K} in the first Friedmann equation (2.4) is justified in being neglected as it is soon redshifted away as a^{-2} , also ordinary matter and radiation are redshifted as a^{-3} and a^{-4} , respectively as shown in equations (2.8) and (2.10).

While the equation of state of ordinary matter does not satisfy (2.27), this situation can be mimicked by a scalar field. The action for a minimally coupled scalar field φ is given by

$$S = \int d^4x \sqrt{-g} \mathcal{L} = \int d^4x \sqrt{-g} \left[\frac{1}{2} g^{\mu\nu} \varphi_{,\mu} \varphi_{,\nu} - V(\varphi) \right]. \quad (2.28)$$

In a FLRW universe described by the Metric (2.1), the equation for φ obtained from (2.28) is

$$\ddot{\varphi} + 3H\dot{\varphi} - \frac{\nabla^2\varphi}{a^2} + V(\varphi)_{,\varphi} = 0. \quad (2.29)$$

Note that the expansion of the universe introduces a friction term in the scalar field equation. The energy-momentum tensor is obtained from the Lagrangian as

$$T_{\mu\nu} = -2\frac{\partial\mathcal{L}}{\partial g^{\mu\nu}} + g^{\mu\nu}\mathcal{L} \quad (2.30)$$

A homogeneous scalar field $\varphi(t)$ (if the $\nabla^2\varphi$ term can be neglected) behaves like a perfect fluid with background energy density and pressure given by

$$\rho_\varphi = \frac{\dot{\varphi}^2}{2} + V(\varphi), \quad (2.31)$$

$$p_\varphi = \frac{\dot{\varphi}^2}{2} - V(\varphi). \quad (2.32)$$

Now, if

$$V(\varphi) \gg \dot{\varphi}^2, \quad (2.33)$$

we obtain

$$p_\varphi = -\rho_\varphi. \quad (2.34)$$

Therefore, if a causally connected patch of the early universe is dominated by the potential energy of a scalar field such that $V(\varphi) \gg \dot{\varphi}^2$ and the initial conditions are such that the field is sufficiently smooth so that the $\nabla^2\varphi$ term can be neglected in (2.29), then there is exponential expansion.

2.2.3 Numerical Example

Next, since it is simple enough and usually not found in cosmology text-books, we consider a simple numerical toy model of a spatially homogeneous scalar field with a quadratic potential. The Friedmann equation (2.4) and the scalar field equation (2.29) read

$$\left(\frac{\dot{a}}{a}\right) = \frac{4\pi G}{3}(\dot{\varphi}^2 + \varphi^2) \quad (2.35)$$

$$\ddot{\varphi} + 3\frac{\dot{a}}{a}\dot{\varphi} + \varphi = 0 \quad (2.36)$$

The solutions of equations (2.35) and (2.36) are shown in figure 2.1. $t_i = 0$ just marks the beginning of

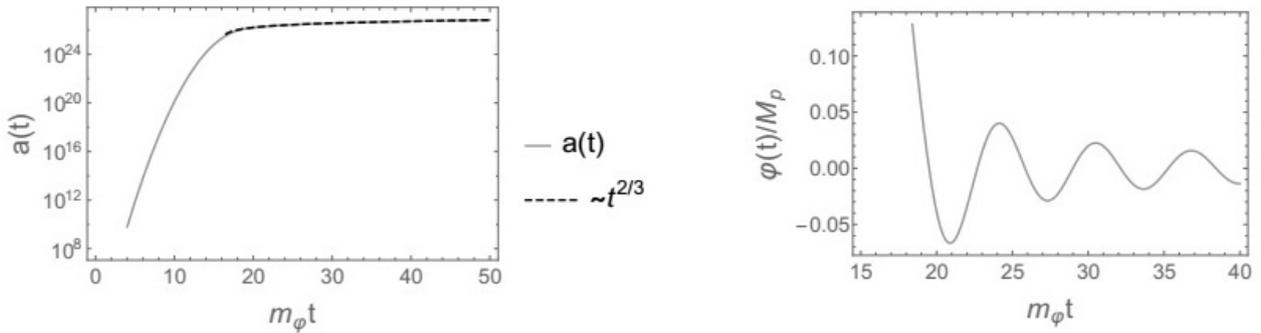


Figure 2.1: *Solutions of equations (2.35) and (2.36) with initial conditions $a_i = 1$, $\varphi_i = 3.06 M_p$ and $\dot{\varphi}_i = 0$. The dashed line corresponds to a dust-dominated expansion, $a(t) \sim t^{2/3}$. In this toy model, inflation ends after ~ 60 e-foldings. The inflaton field starts decaying slowly, linearly and then it begins damped oscillations. At the end of inflation, a mechanism like reheating is necessary to smoothly connect the scenario to the radiation-dominated phase of the standard model [34, 35].*

inflation, having nothing to do with a beginning of physical time. Inflation starts as the energy of the inflaton field is dominated by its slowly decaying potential. At some point, the potential stops dominating and inflation ends, when the scalar field starts oscillating. The scale factor grows about 10^{26} times during inflation in this toy model and the universe is left in a cold, dust-like dominated expansion.

The initial conditions in this toy model, with the inflaton field energy near the Planck mass, cast doubts on the applicability of the classical equations of motion. This is representative of a family of models called large-field inflation. More generally, the problem of the robustness of the predictions with respect to full quantum gravity effects needs to be addressed in any model of the very early universe, but it is specially important in the inflationary scenario because its initial conditions are placed in a high energy density regime.

2.2.4 (P)reheating After Inflation

After inflation, the universe is left in a cold, low density, dust-like dominated expanding state. An extra mechanism is therefore necessary to smoothly connect the end of inflation to the hot big bang phase so that the predictions of the standard model, in agreement with observations, are not spoiled. This mechanism is generally called reheating [34–36]. Since all kinds of energy (except quantum fluctuations) present before inflation are diluted away, almost all the matter is created at that time and this is also where baryogenesis takes place.

The first stage of reheating is a non-perturbative process of quantum particle creation called preheating. This is similar in spirit to gravitational particle creation and the creation of pairs by electromagnetic fields, more generally it is creation of particles from an external classical source. The fields, whose particles are created, interact with the classical coherently oscillating inflaton field resulting in a Mathieu-like differential equation [37]. For certain values of the parameters in a given range, there is parametric resonance which greatly enhances

particle creation. In general, however, there is no explanation as to why these parameters should be in a resonant configuration. If there is resonance, it takes only a few oscillations to deplete the energy of the inflaton field.

The non-perturbative nature of preheating allows, for instance, the copious production of superheavy particles with masses greater than the inflaton mass (~ 13 GeV), which is clearly forbidden in a perturbative regime. This issue is important because interactions and decay of such heavy particles may lead to baryogenesis in grand unified theories. On the other hand, there is also the danger of overproduction of gravitons which could in principle close the universe before nucleosynthesis takes place, and of neutrinos which could also spoil the predictions of nucleosynthesis.

After preheating the particles interact among themselves and slowly decay after which follows an eventual thermalization. This can be treated within perturbation theory as described in [38]. The final temperature obtained, constrained by the temperature at the primordial nucleosynthesis, is determined by the strength of the couplings of the inflaton field to the other fields, which makes it model dependent. The necessity of new parameters and models of interactions of course weakens the predictability of the scenario.

As a final remark, in the bouncing scenario the hot big bang phase after the bounce follows by construction if there was a radiation dominated phase before the bounce, resulting in a nearly symmetric bounce. It is still necessary to explain why it should be so, but the point is that reheating is not strictly required although particle creation is not forbidden either. It is important though to investigate if the bounce is stable against cosmological perturbations or particle creation.

2.3 Bouncing Cosmology

The bouncing cosmology paradigm [1–3, 20–22] is a theoretical framework according to which the standard big bang expansion is preceded by a phase of contraction. The scale factor starts at a huge classical value, where the initial conditions are placed, and then shrinks up to a minimum at the bounce before growing again into the standard hot Big Bang phase. It is a very general idea that can be implemented in many ways and, just as inflation but from a different perspective, it may solve the cosmological puzzles in the standard model and produce an almost scale invariant spectrum of perturbations.⁷

The *raison d'être* of the bouncing paradigm is to avoid the initial singularity. The use of classical general relativity to describe the standard model of cosmology implies that there was in a finite past, some 13.8 billion years ago, a so called big bang singularity: a regime where physical variables, such as the strength of the gravitational field, go to infinity. Singularities in general relativity [39] are even worse than those found in quantum field theory for they are not regarded as part of the physical, real space-time and physics laws can only work in the realm of space-time. The standard model (including inflation [33]) thus imply that the universe started in a state that cannot even in principle be described by the laws of physics, a source of lawlessness [1, 25], which is of course not acceptable.

2.3.1 Issues in the Inflationary Picture

The persistence of long standing issues in the inflationary picture may cast doubts on its reality and motivates the search for alternatives. Some of these problems are listed below.

Singularity

Even though the inflaton field does not satisfy the energy conditions of the singularity theorems of the 1960s, it has been shown that a past singularity is still unavoidable in the inflationary context [33]. Therefore, scalar field driven inflation cannot be the ultimate theory of the early universe.

⁷We consider only bouncing models that are not followed by inflation for they are more interesting from the point of view of observations.

Trans-Planckian Window

If the period of inflation lasted sufficiently long, then all scales inside the Hubble radius today started out with a physical wavelength smaller than the Planck scale at the beginning of inflation. It is unclear how the predictions of inflation are robust with respect to quantum gravity effects.

Particle Physics Motivation

This concerns the nature of the inflaton field. The required properties of the potential to yield inflation are not well motivated by fundamental particle physics theory. In general, it is necessary to invoke super-symmetry and even then special initial conditions are required.

Energy Scale of Inflation

The energy scale at which inflation takes place may be too high to justify the use of classical general relativity. In simple toy models, the energy scale during inflation is very close to the Planck scale, where the classical notion of space-time is in check. In fact, in large field models the initial amplitude of the scalar field may be even higher than the Planck energy.

Measure Problem

It turns out that essentially all inflationary models are eternal which leads to the notion of a multiverse. It means that inflation never ends globally, only locally. The inflating region grows exponentially without limit, while pieces of it break off to form "bubble" universes. This makes it difficult to extract meaningful predictions.

Uniqueness of Observations

Contrary to what is usually advertised, the observed patterns in the CMBR at the current precision level are not uniquely explained by inflation; some alternative models can also do the job. This remark alone should be reason enough to pay some attention to these alternatives.

2.3.2 Classical Bounce

At the classical level, the possibility of a bouncing universe is determined by the Einstein equations. Since the Hubble rate is negative during the contracting phase, while it is positive during the subsequent expanding phase, the bounce must allow the Hubble rate to increase so that $\dot{H} > 0$. The Friedmann equations (2.4) and (2.5) may be combined to show that

$$\dot{H} = -\frac{1}{2}(\rho + p) + \frac{\mathcal{K}}{a^2}. \quad (2.37)$$

Note that general relativity forbids a flat ($\mathcal{K} = 0$) FLRW bouncing universe dominated by a fluid that respects the null energy condition (NEC), $\rho + p > 0$, at the bouncing phase.

Moreover, note that the condition

$$p < -\rho. \quad (2.38)$$

is even stronger than (2.27). It may thus be argued that the bouncing paradigm is even more exotic than inflation. There must be either an exotic fluid that violates the NEC, or modifications to the Einstein equations that act effectively as repulsive gravity. These modifications may be due to additional terms in the classical Lagrangian of gravity or due to quantum gravitational effects.

Solution of the Standard Puzzles in the Bouncing Scenario

Horizon: The existence of a singularity in the past, a beginning of time, implies that there is a finite distance that light may have travelled since then. This is called the horizon. The size d_H of the horizon is given by the time integral $d_H(t) \equiv a(t) \int_{t_i}^t a^{-1}(\tau) d\tau$, where t_i is the initial time (we assume for simplicity that the bounce takes place at $t = 0$, so that $t < 0$ represents the contracting phase and $t > 0$, the expanding phase). Assuming that the dynamics is driven by a perfect fluid with constant equation of state, we can use equation (2.17) to calculate the horizon

$$d_H(t) = \frac{3(1+\omega)}{1+3\omega} \left[|t_i|^{\frac{1+3\omega}{3(1+\omega)}} - |t|^{\frac{2}{3(1+\omega)}} + t \right]. \quad (2.39)$$

If $\omega > -1/3$, as $t_i \rightarrow \infty$ (in the bouncing scenario), the horizon d_H diverges. At any finite time before or after the bounce, the horizon is infinite. Note that this solution requires $\omega > -1/3$ so that the universe was not dominated by some kind of dark energy in the contracting phase, as is the case in the present expanding phase. It thus appears to require a nonsymmetric bounce.

Flatness: The flatness problem refers to the fact that the curvature contribution to the Friedmann equation (2.4) is unstable in the standard model (it grows with time)

$$\frac{d}{dt} |\Omega - 1| = -\frac{\dot{a}^3}{\ddot{a}}, \quad (2.40)$$

Given that Ω is observed to be close to unity today, it must be fine-tuned in the past in a radiation- or a dust-dominated expansion. In the bouncing scenario, this is solved through a decelerated contracting phase, $\ddot{a} < 0$ and $\dot{a} < 0$, such that the curvature contribution decreases with time. The universe is thus seen to be almost flat now because it has expanded much less than it has contracted before.

2.3.3 Advantages of the Bouncing Scenario

Some of the advantages of the bouncing picture are summarized in the list below.

Absence of Singularity

The bouncing scenario solve the initial singularity problem by construction, meaning that the scale factor stops contraction at a finite value so that the density does not reach arbitrarily high values.

Cosmological Puzzles

It may solve the cosmological puzzles, just as inflation but from a different perspective.

Trans-Planckian Window

The initial conditions may be placed in a classical coherent state in the past contracting phase away from the bounce so that the trans-Planckian window is a non issue at least in semi-classical models.

Particle Physics

It does not rely on any extension of the standard model of particle physics; in particular it does not require supersymmetry, although it does not forbid it either. It does not even require a scalar field, although it does

require some new physics. To be fair, note that (2.38) is a stronger requirement than (2.27). In that sense, the bouncing scenario can be considered to be more exotic than inflation.

Classical and Quantum Gravity

It can be embedded in all the known paradigms of classical and quantum gravity, including the most popular ones: superstring theory and loop quantum gravity. The bouncing scenario seems to be a general prediction of the latter [40]. However, string theory seems to favor the inflationary scenario [19, 41].

Observations

It may give rise to a scale invariant spectrum of scalar perturbations in accord with observations, which is the motto of inflationary theory practitioners.

Falsifiability

The specific models in the bouncing paradigm may have clear distinct predictions from inflation [3, 42]: the tensor ratio, the index running, non-Gaussianities. Therefore, they can be falsified in future observations.

2.3.4 Scale-Invariant Spectrum

In this section, we sketch a simple demonstration that a matter dominated contracting universe can give rise to a scale invariant spectrum of perturbations. In this toy model, matter is modeled by some scalar field φ in a gravitational field with total action given by

$$S = -\frac{1}{16\pi G} \int d^4x \sqrt{-g} R + \int d^4x \sqrt{-g} \left[\frac{1}{2} g^{\mu\nu} \varphi_{,\mu} \varphi_{,\nu} - V(\varphi) \right]. \quad (2.41)$$

The background equations of motion for the scale factor and for the scalar field are, respectively,

$$H^2 = \left(\frac{\dot{a}}{a} \right)^2 = \frac{8\pi G}{3} \left[\frac{1}{2} \dot{\varphi}^2 + V(\varphi) \right] \quad \text{and} \quad \ddot{\varphi} + 3H\dot{\varphi} + V_{,\varphi} = 0, \quad (2.42)$$

which can be combined to show that

$$\dot{H} = -4\pi G \dot{\varphi}^2. \quad (2.43)$$

Since matter and gravitational perturbations, respectively $\delta\varphi$ and Φ , are related by the Einstein equations, they can be combined into a single variable v , called the Mukhanov–Sasaki variable [43], which is a gauge-invariant potential given by

$$v = a \left(\delta\varphi + \frac{z}{a} \Phi \right), \quad (2.44)$$

where z determines the time-dependent mass scale of v and is given by

$$z = \frac{a\varphi'_0}{\mathcal{H}}. \quad (2.45)$$

The equations of motion for the Fourier modes of the Mukhanov–Sasaki variable are [43]

$$v_k'' + \left(k^2 - \frac{z''}{z} \right) v_k = 0. \quad (2.46)$$

In the case of a matter dominated phase of contraction, the scale factor is $a \sim t^{2/3} \sim \eta^2$ so that $\mathcal{H}' \sim \mathcal{H}^2$. Equation (2.43) written in conformal time can then be used together with (2.45) to show that $z \sim a$, which is also valid in the more general case of a time-independent background equation of state. Hence, the negative square mass term in (2.46) is \mathcal{H}^2 . Therefore, on length scales smaller than the comoving scale, $k \gg \mathcal{H}$, the solutions for v_k are constant amplitude oscillations, so these modes are stable. On super-Hubble scales, $k \ll \mathcal{H}$, the solutions are frozen in as standing waves, and their amplitude depend on the time evolution of z ; equation (2.46) for v_k gives

$$v_k(\eta) = c_1 \eta^2 + c_2 \eta^{-1}, \quad (2.47)$$

where c_1 and c_2 are constants. The c_1 mode is the mode for which the physical perturbations, v_k/a , are constant on super-Hubble scales. In a contracting phase, it is the c_2 mode which dominates and leads to a scale-invariant spectrum

$$P_\zeta(k, \eta) \sim k^3 |v_k(\eta_H(k))|^2 \left(\frac{\eta_H(k)}{\eta} \right)^2 \sim \text{const}, \quad (2.48)$$

where vacuum conditions are given at the Hubble crossing, $\eta_H(k) \sim k^{-1}$ and $v_k \sim k^{-1/2}$.

In the bouncing scenarios, it is necessary to show that the scale-invariant spectrum obtained in the contracting branch survives to the expanding branch in order to fit observations. This is a difficult task, since it is expected that quantum gravity effects may become important at the bouncing phase, precluding the use of classical general relativity. The solution to this issue, which may be referred to as matching conditions, depend on the physics that drives the cosmic bounce. In some cases, the scale-invariant spectrum is known to be preserved.

To conclude this section, note from the dominant term of (2.47) that the physical amplitude of the pertur-

bations are $v_k/a \sim a^{-3/2} \sim t^{-1}$, and their kinetic energy density is roughly

$$\left(\frac{d}{dt} \frac{v_k}{a}\right)^2 \sim \frac{1}{t^4} \sim \frac{1}{a^6}. \quad (2.49)$$

Therefore the energy density of the perturbations grows as fast as a^{-6} which is faster than non-relativistic matter and radiation. The perturbations may then eventually dominate and destroy the homogeneous bounce, which renders the model unstable. This is called the Belinsky–Khalatnikov–Lifshitz instability. Since the constants of integration have been ignored, it may be argued that this is really a matter of initial conditions: using the observed density parameters to estimate the relative importance of the perturbations at the contracting phase, it can be shown that this is not necessarily a fine-tuning problem. Note that the quantum cosmological model that we consider later is effectively stiff-matter-dominated at the bounce, $\rho \sim a^{-6}$. In this particular case, this is clearly a matter of initial conditions.

Chapter 3

Quantum Cosmological Bounce in the de Broglie-Bohm Theory

Deep in the human unconscious is a pervasive need for a logical universe that makes sense. But the real universe is always one step beyond logic.

Frank Herbert, *Dune*.

A definitive answer to the problem of the initial singularity cannot be given without a fully consistent quantum theory of gravity. In the meantime, one can only hope that one of the existing approaches may give a solution close to what is realized in the early universe. Since these approaches are constructed with low energy physics as an effective limit, it might not be wishful thinking to expect so. It is certainly possible that quantum gravity turns out to be something completely new, but even then it would have to satisfy low energy constraints.

Currently, the most popular approach to quantum gravity is super-string theory [44, 45]. Starting with the seemingly simple idea that particles are actually strings, it has far reaching consequences both for gravitation and cosmology [19, 41]. If it turns out to be correct, it will be another revolution in the understanding of space-time. In particular, it predicts (more accurately, requires) that space-time has more than the usual 4 dimensions. Another important feature is that it treats gravity and particle physics in the same framework.

Another interesting and popular approach to quantum gravity is loop quantum gravity [46, 47]. This is an approach that is both more modest and more conservative than string theory. It is more modest because it deals only with gravity. It is more conservative because it comes from an Hamiltonian approach to general relativity. An interesting prediction of LQG is that space can be fundamentally divided in atoms of space. As a

consequence, space behaves as a sponge that can only absorb a limited amount of water (energy), and gravity becomes repulsive beyond that limit [40]. Thus, the bouncing scenario seems to be a general prediction of LQG.

In this chapter, however, we follow a less popular approach [2] that is based on the de Broglie–Bohm interpretation of quantum mechanics [48–51] applied to the Wheeler-deWitt equation [52], which is expected to work up to the Planck scale, in mini-superspace. It makes no assumptions on the quantum nature of space–time, except that the commutation relations must be consistent with the classical Hamiltonian constraints. It gives a well defined trajectory for the scale factor, not just an expectation value for some operator that would describe the volume of space. The scale factor thus obtained can be used as a simple c-number in other dynamical equations, without any quantum–mechanical ambiguities.

3.1 Quantum Cosmology

The subject of quantum cosmology is an attempt to apply the principles of quantum mechanics to the universe as a whole, with the hope to renormalize the initial singularity. The expression "quantum cosmology" seems a bit paradoxical, as cosmology is a very large scale science and quantum mechanics is supposed to govern small quantum systems. However, there has been over the years a growing consensus that quantum theory should be a universal theory of nature. In that sense, all classical systems emerge from some set of quantum laws. This is the case in early universe cosmology, as the singularity in the standard model seems to imply. In this section, we briefly sketch the canonical approach to quantum cosmology. This is by far the most conservative method among the attempts to quantize gravity.¹ This is based on an approach pioneered by Dirac to the quantization of constrained systems [55]. The constraints, in our case, are the Hamiltonian constraints of general relativity.²

3.1.1 Classical Hamiltonian Formalism

An inspection of the Einstein equations show that only the spatial part of the metric, h_{ij} , appear with second order time derivatives. These are thus the dynamical variables of general relativity. The other components of the metric are constraints. The presence of constraints shows not only that initial values cannot be chosen arbitrarily, but also that there are underlying symmetries. Constraints of a certain type called first class, as they are realized in general relativity, generate gauge transformations. Classically, the gauge transformations of general relativity are equivalent to coordinate changes. Gauge invariance thus implies the general covariance under coordinate changes.

In the Hamiltonian formulation of general relativity, it is assumed that space–time can be split into a family of space–like hypersurfaces and a time–like direction. Thus, the topology of the manifold is restricted to $M^4 = \mathbb{R} \times \mathcal{M}^3$. This excludes space–times with rotations and pathologies such as closed time–like curves. The non–intersecting space–like hypersurfaces can be defined by the equations $\phi(x^\mu) = \text{constant}$. The vector $\eta_\mu = \phi_{,\mu}$ is normal to the hypersurface, because the value of ϕ can only change in the orthogonal direction. Since these hypersurfaces are space–like, they can be parameterized by a time–like coordinate $x^0 = t$ yielding $\eta_\mu = \delta_\mu^0$, where N is a normalization factor. $g^{\mu\nu}g_{\mu\nu} = -1$ implies that $g^{00} = -1/N^2$. The projector onto the hypersurfaces is given by $h^{\mu\nu} = g^{\mu\nu} + \eta^\mu\eta^\nu$, whose components are $h^{00} = 0$, $h^{0i} = 0$ and $h^{ij} = g^{ij} + N^2g^{0i}g^{0j}$.

¹We will not be concerned with claims that this approach is not renormalizable for two reasons: first, because this method may be seen as an effective approach with a cut-off near the Planck scale; second, because there are examples of exactly solvable non-perturbative theories in which the perturbation expansion is not renormalizable [53] (see also the introduction in [54]). We take the former point of view, which is safer.

²A useful introduction to the purely classical Hamiltonian formulation of GR can be found in [56].

Assuming the 3 + 1 decomposition, the metric can thus be written in the ADM form

$$\begin{aligned}
ds^2 &= g^{\mu\nu} dx^\mu dx^\nu \\
&= (N_i N^i - N^2) dt^2 + 2N_i dx^i dt + h_{ij} dx^i dx^j \\
&= N^2 dt^2 + h_{ij} (N^i dt + dx^i) (N^j dt + dx^j)
\end{aligned} \tag{3.1}$$

The lapse function $N(t, x^k)$ is the rate of change with respect to the coordinate time t of the proper time of an observer with 4-velocity $\eta_\mu(t, x^k)$. The shift function $N^i(t, x^k)$ is the rate of change of the shift of the points with the same label x^i from one hypersurface to another with respect to coordinate time t . The shift function can also be viewed as the projection of the tangent vector $\partial/\partial t$ to the t -time coordinate curves onto the spacelike hypersurface.

A hypersurface characterized by the metric h_{ij} has its own curvature associated with its 3-geometry that can be calculated in the usual way. However, another quantity is necessary to define how these 3-dimensional hypersurfaces are curved with respect to the 4-dimensional manifold in which they are immerse, so that the spacetime foliation is uniquely defined. This is the extrinsic curvature. It compares the normal vector η_μ at one point with the parallel transported normal vector from a neighboring point

$$K_{\mu\nu} = -h_\mu^\alpha h_\nu^\beta \nabla_{(\alpha} \eta_{\beta)}, \tag{3.2}$$

with $h_\mu^\alpha = \delta_\mu^\alpha + \eta^\alpha \eta_\mu$ the projector onto the hypersurface at which η^μ is normal and $\nabla_\alpha \eta_\beta = \eta_{\beta,\alpha} - \Gamma_{\alpha\beta}^\gamma \eta_\gamma$ is the covariant derivative of η^μ . The relevant components are

$$\begin{aligned}
K_{ij} &= -N \Gamma_{ij}^0 \\
&= \frac{1}{2N} \left[2D_{(i} N_{j)} - \frac{\partial h_{ij}}{\partial t} \right],
\end{aligned} \tag{3.3}$$

where D_i is the 3-dimensional (intrinsic) covariant derivative with respect to h_{ij} .

Using these definitions, the 4-dimensional Ricci scalar can be written in terms of the 3-geometry as [56, 57]

$$R = R^{(3)} + K^{ab} K_{ab} + K^2 - \frac{2}{N} \partial_t K + \frac{2N^i}{N} \partial_i K - \frac{2}{N} D_i (\partial^i N), \tag{3.4}$$

where $R^{(3)}$ is the 3-dimensional Ricci scalar. After discarding surface terms, the Einstein-Hilbert Lagrangian density becomes

$$\mathcal{L} [N, N^i, h^{ij}] = N \sqrt{h} \left(R^{(3)} + K^{ab} K_{ab} - K^2 \right). \tag{3.5}$$

Since the Lagrangian density (3.5) does not depend on $\partial_t N$ nor on $\partial_t N^i$, their canonical conjugate momenta

are constraints [55, 58, 59]

$$\Pi = \frac{\delta L}{\delta(\partial_t N)} \approx 0, \quad (3.6)$$

$$\Pi_i = \frac{\delta L}{\delta(\partial_t N^i)} \approx 0. \quad (3.7)$$

(3.6) and (3.7) are called primary constraints. The canonical momenta conjugate to h^{ij} is

$$\Pi_{ij} = \frac{\delta L}{\delta(\partial_t h^{ij})} = -\sqrt{h}(K_{ij} - h_{ij}K). \quad (3.8)$$

The Hamiltonian density is

$$\mathcal{H} = \Pi_{ij}\partial_t h^{ij} - \mathcal{L}, \quad (3.9)$$

and the Hamiltonian is

$$H = \int d^3x \mathcal{H} = \int d^3x (N\mathcal{H} + N_j \mathcal{H}^j), \quad (3.10)$$

with

$$\mathcal{H} = G_{ijkl}\pi^{ij}\pi^{kl} - \sqrt{h}R^{(3)}, \quad (3.11)$$

$$\mathcal{H}^j = -2D_i\pi^{ij}, \quad (3.12)$$

where G_{ijkl} is the DeWitt metric

$$G_{ijkl} = \frac{1}{2\sqrt{h}}(h_{ik}h_{jl} + h_{il}h_{jk} - h_{ij}h_{kl}). \quad (3.13)$$

For consistency, the primary constraints must be conserved in time, $\dot{\pi}_\mu = \{\pi_\mu, \mathcal{H}\} = 0$. This implies the weak equations

$$\mathcal{H} \approx 0, \quad (3.14)$$

$$\mathcal{H}^j \approx 0. \quad (3.15)$$

The equations (3.14) and (3.15) are secondary constraints called super-Hamiltonian and super-momentum constraints, respectively. They are closely tied with general covariance and their conservation in time do not lead to new constraints. The equation (3.14) leads to the problem of time after quantization. Since N and N^i have no dynamics and multiply secondary constraints in the Hamiltonian (3.10), they can be seen as the Lagrange multipliers of these constraints, and they may be eliminated from the phase space of the theory.

The secondary constraints (3.14) and (3.15) have weakly zero Poisson brackets among each other. They are

called first-class constraints. The Dirac conjecture, proven in [60], states that all first-class are generators of gauge transformations. In the case of the super-Hamiltonian and the super-momentum constraints, it can be shown that [58]

$$\delta h_{ij}(x) = \left\{ h_{ij}(x), \int d^3y \zeta(y) \mathcal{H}(y) \right\} = -2\zeta(x)K_{ij}(x) = \zeta(x)\mathcal{L}_\eta h_{ij}, \quad (3.16)$$

$$\delta h_{ij}(x) = \left\{ h_{ij}(x), \int d^3y \xi^k(y) \mathcal{H}_k(y) \right\} = D_i \xi_j(x) + D_j \xi_i(x) = \mathcal{L}_\xi h_{ij}, \quad (3.17)$$

where where \mathcal{L}_ξ is the Lie derivative along the infinitesimal space-like vector ξ and \mathcal{L}_η is the Lie derivative along the direction orthogonal to the space-like hypersurfaces with metric h_{ij} . The function $\zeta(x)$ is infinitesimal. Analogous results can be obtained for the momenta π_{ij} . The super Hamiltonian constraint (3.14) is the generator of time reparametrization. As can be seen from equation (3.16), (3.14) is connected to time evolution. The super momentum constraints (3.15) are the generators of spatial coordinate transformations.

3.1.2 Quantization of the Hamiltonian Constraints

According to the Dirac quantization procedure, physical states are annihilated by the operator representations of the classical constraints, where

$$h_{ij} \rightarrow \hat{h}_{ij} \quad \text{and} \quad \pi^{ij} \rightarrow -i \frac{\delta}{\delta h_{ij}}, \quad (3.18)$$

and the wavefunction must satisfy a Schrödinger-like functional equation

$$i \frac{\partial \Psi}{\partial t} = H \Psi, \quad (3.19)$$

where H is the operator obtained from the classical Hamiltonian (3.10). The superspace constraints (3.14) and (3.15) become

$$\mathcal{H} \Psi = 0, \quad (3.20)$$

$$\mathcal{H}^j \Psi = 0. \quad (3.21)$$

The equations (3.20) and (3.21) imply that the right-hand side of equation (3.19) is zero, which means that Ψ does not depend on time. This is also true in the presence of matter.

The momentum constraint (3.21) implies that the wavefunction is invariant with respect to spatial coordinate transformations on the three-surface. To see this, consider the effect of a diffeomorphism $x^i \rightarrow x^i - \xi^i$ on the

three-surface [61]

$$\delta\Psi = \Psi [h_{ij} + D_{(i}\xi_{j)}] - \Psi [h_{ij}] = \int d^3x D_{(i}\xi_{j)} \left(\frac{\delta\Psi}{\delta h_{ij}} \right) = - \int d^3x \xi_j D_i \left(\frac{\delta\Psi}{\delta h_{ij}} \right) = \frac{1}{2i} \int d^3x \xi_i \mathcal{H}^i \Psi = 0, \quad (3.22)$$

where the third equality follows from integration by parts and the boundary term is assumed to vanish; and the last equality follows from the super momentum constraints (3.21). Therefore, the wavefunction is a functional of an equivalence class of metrics which describe the same geometry, not of one particular metric. The space of all three-dimensional space-like geometries is called superspace.

The equation (3.20) is called the Wheeler–DeWitt equation. Using equation (3.11), it can be written as

$$\left[G_{ijkl} \frac{\delta}{\delta h_{ij}} \frac{\delta}{\delta h_{kl}} - \sqrt{h} R^{(3)} + \mathcal{H}_{\text{matter}} \right] \Psi = 0. \quad (3.23)$$

Note that this contains products of local operators acting on the same "point", therefore it must be regularized. There is also a factor ordering issue, just as in the usual non-relativistic quantum mechanics. The equation (3.23) is therefore only formal at this stage. The issue of time [62, 63] refers to the remark previously made that Ψ does not depend on cosmic time. A possible solution is to introduce a perfect fluid with a constant equation of state [2]. The momentum $-i\delta/\delta\varphi$ conjugate to the fluid variable φ appears linearly in the matter contribution to the Hamiltonian in (3.23) [64, 65]. This makes it possible to write down the Wheeler-DeWitt equation in a Schrödinger-like form. The fluid variable φ may therefore play the role of time.

The fact that the gravitational Hamiltonian is not bounded from below also has implications for quantum gravity. In particular, a perturbative approach based on such Hamiltonian is rendered unstable. However, as an effective theory (3.23) is expected to be a useful approximation up to the Planck energy scale.

3.1.3 Minisuperspace Models

The Wheeler–DeWitt equation (3.23) is a complicate functional differential equation, which is equivalent to a system of partial differential equations for each space point. Such a system is pathological and impossible to solve in general. However, one would like to investigate issues related to the quantization of the universe, such as the singularity problem in classical cosmology, more deeply. Hence, it should be a good strategy to get rid of the difficult technical problems characteristic of the Wheeler–DeWitt equation in full superspace, and work in a more restricted framework while hoping that the essential features of quantum cosmology remain. Furthermore, the great degree of space homogeneity of the primordial universe suggests that this simplification can be physically reasonable when dealing with quantum cosmology.

In order to do that, one simplifies the Wheeler–DeWitt equation by freezing out degrees of freedom of gravity

and matter, reducing the superspace to a minisuperspace where only a finite amount of the degrees of freedom are still available. A minisuperspace is the set of spacelike geometries and matter fields where all but a finite set of the canonical variables and their corresponding momenta are set to zero. Evidently, this violates the uncertainty principle. However, we expect that the quantization of these minisuperspace models retains many of the qualitative features of the full quantum theory, which are easier to study in these simplified models.

3.2 de Broglie–Bohm Quantum Cosmology

The de Broglie–Bohm interpretation of quantum mechanics [48–51], also referred to as the causal interpretation, the quantum theory of motion, and sometimes the ontological interpretation, is an alternative description of quantum processes as opposed to the usual standard view of the Copenhagen interpretation of quantum mechanics. The main points in the general philosophical view adopted in the de Broglie–Bohm interpretation are that quantum processes are real, objectively existing physical processes which take place independently of conscious observers (or an external system to which quantum theory does not apply), and that the quantum theory can describe individual processes as opposed to being restricted to the description of ensembles. It is thus an appealing framework if quantum theory is to be regarded as universal.

3.2.1 Why Not Copenhagen?

As explained in [2] (and references therein), the Copenhagen interpretation of quantum mechanics [66], the orthodox one usually taught in text–books and standard undergraduate courses, cannot make sense as a quantum theory of the universe. A central feature is that it assumes from the start the existence of a classical domain outside the observed quantum system and not subject to quantum laws. Moreover, objective reality seems to be intricate with the notions of observer and measurement. For example, questions related to physical quantities prior to a measurement are often disregarded as meaningless. The measurement process randomly picks out exactly one of the many possibilities allowed by the wavefunction in such a way that probability has a fundamental (as opposed to emergent) status. The interaction of an external observer or apparatus to the quantum system causes the wavefunction to collapse. Since the collapse of the wavefunction can not be described as a unitary evolution according to the Schrödinger equation, and there is no superposition in the final state of the apparatus so that the measurement is robust, it follows that the measurement takes place outside the quantum world with an apparatus not subject to quantum laws. Note that these features are directly opposite to the widely spread belief among the scientific community that quantum theory is a universal and fundamental theory, applicable to any physical system, from which classical physics can be recovered. Moreover, the necessity of an external classical domain precludes the application of the Copenhagen interpretation as it stands as a quantum theory of the universe.

Some approaches to this problem are summarized in [2]. Here, we are interested in an alternative approach, the de Broglie–Bohm interpretation of quantum mechanics. The splitting of the wavefunction is explained as follows. A point–particle in configuration space describing the observed system and apparatus is objectively real, meaning that it exists by itself, it has an ontological status that does not depend on observations. In the

splitting, this point particle enters into one of the wavefunction branches (depending on the initial position of the point particle before the measurement, which is unknown) and the other branches will be empty. The empty waves can neither interact with other particles, nor with the point particle containing the apparatus. This looks effectively as a collapse of the wavefunction but the empty branches continue to exist. Schrödinger evolution is always valid, and there is no artificial division between classical and quantum worlds. This is thus suitable to quantum cosmology.

3.2.2 de Broglie–Bohm Interpretation

The best way to introduce the de Broglie–Bohm interpretation of quantum mechanics is through the example of a quantum particle. Let $\Psi(t, x)$ be the wavefunction of a non-relativistic particle. The Schrödinger equation in coordinate representation reads

$$i\hbar \frac{d}{dt} \Psi(t, x) = \left[-\frac{\hbar^2}{2m} \nabla^2 + V(x) \right] \Psi(t, x). \quad (3.24)$$

Writing $\Psi = R \exp(iS/\hbar)$ in (3.24) results in the following equations

$$\frac{\partial S}{\partial t} + \frac{(\nabla S)^2}{2m} + V - \frac{\hbar^2}{2m} \frac{\nabla^2 R}{R} = 0, \quad (3.25)$$

$$\frac{\partial R^2}{\partial t} + \nabla \cdot \left(R^2 \frac{\nabla S}{m} \right) = 0. \quad (3.26)$$

The basic postulates of the de Broglie–Bohm interpretation are [2, 49]

1. An individual physical system comprises a wave propagating in space and time together with a point particle which moves continuously under the guidance of the wave.
2. The wavefunction is a solution to the Schrödinger wave equation.
3. The particle motion is obtained as the solution $x(t)$ to the equation

$$\dot{x} = \frac{\nabla S}{m} \quad (3.27)$$

This is the so-called guidance equation. The precise trajectory depends on the initial condition $x(t_0) = x_0$, which is however unknown. An ensemble of possible motions associated with the same wave is generated by varying x_0 .

4. Equation (3.25) is an Hamilton–Jacobi equation for a particle submitted to an external potential which

is the classical potential plus a new quantum potential

$$Q = -\frac{\hbar^2}{2m} \frac{\nabla^2 R}{R}. \quad (3.28)$$

Hence, the particle trajectory $x(t)$ satisfies the equation of motion

$$m\ddot{x} = -\nabla V - \nabla Q. \quad (3.29)$$

Note that the quantum potential is present even when the classical potential vanishes.

5. In a statistical ensemble, if the probability density for the unknown initial position is given by $P(x_0) = R^2(t = t_0, x = x_0)$, equation (3.26) guarantees that $R^2(t, x)$ gives the distribution of positions at any time, and all statistical predictions of quantum mechanics are recovered.

Note from equation (3.28) that the quantum potential depends only on the shape of Ψ , not on its absolute value. Also, it is clearly non-local in systems with many particles. This is consistent with the Bell inequalities, which show that a quantum theory must be either non-local or non-ontological. The quantum potential is responsible for the quantum effects. Note that even a classically free particle may be subject to a non-vanishing quantum potential. The classical limit is obtained when $Q \approx 0$ compared with the classical kinetic and potential energy terms. Note also that the definition of an individual physical system is not restricted to atomic or subatomic particles [49]. It applies to all matter, regardless of scale, although the wave aspect is generally apparent only in phenomena involving microscopic particles. There is no arbitrary division into subject and object, or observer and observed: it applies to the world as a whole.

3.3 Bouncing–Solutions

In the next subsections, we briefly sketch how the Bohmian trajectories for the scale factor are obtained in the case of a single perfect fluid, and later in the case of a two–components perfect fluid. The way these solutions are obtained is not essential for the calculations of the Bogoliubov coefficients for particle creation in these models. However, it is important that according to the de Broglie–Bohm interpretation these solutions are simply c -numbers, even when the scale factor approaches the minimum value near the bounce. Therefore, the scale factor introduces no operator related complications in the field equations.

3.3.1 Single Fluid

The total minisuperspace Hamiltonian for a single perfect fluid with equation of state $p = \lambda\rho$ in a flat FLRW universe reads [2]

$$H = N \left[-\frac{p_a^2}{4a} + \frac{p_T}{a^{3\lambda}} \right], \quad (3.30)$$

where a is the scale factor, and T represents the degree of freedom associated to the fluid, which will play the role of time. The Wheeler-DeWitt equation (3.20) (with $N = a^{3\lambda}$, for convenience) reads

$$i \frac{\partial \Psi(a, T)}{\partial T} = \frac{1}{4} \frac{\partial^2 \Psi(a, T)}{\partial \chi^2}, \quad (3.31)$$

where

$$\chi = \frac{2}{3} (1 - \lambda)^{-1} a^{3(1-\lambda)/2}. \quad (3.32)$$

This is just the time–reversed one-dimensional Schrödinger equation for a free particle constrained to the positive axis. Since a and χ are positive, unitary evolution implies

$$\left(\Psi^* \frac{\partial \Psi}{\partial \chi} - \Psi \frac{\partial \Psi^*}{\partial \chi} \right) \Big|_{\chi=0} = 0. \quad (3.33)$$

We take a Gaussian wavepacket as the initial normalized wave function,

$$\Psi_i(\chi) = \left(\frac{8}{\pi T_b} \right)^{1/4} \exp \left(-\frac{\chi^2}{T_b} \right), \quad (3.34)$$

where T_b is an arbitrary constant. Ψ_i satisfies the condition (3.33). Using the propagator procedure explained in [67, 68], we obtain the wave solution for all times

$$\begin{aligned} \Psi(a, T) = & \left[\frac{8 T_b}{\pi (T^2 + T_b^2)} \right]^{1/4} \exp \left[-\frac{4 T_b a^{3(1-\lambda)}}{9 (T^2 + T_b^2) (1-\lambda)^2} \right] \\ & \times \exp \left\{ -i \left[\frac{4 T a^{3(1-\lambda)}}{9 (T^2 + T_b^2) (1-\lambda)^2} + \frac{1}{2} \arctan \left(\frac{T_b}{T} \right) - \frac{\pi}{4} \right] \right\}. \end{aligned} \quad (3.35)$$

Due to the chosen factor ordering (momentum to the left), the probability density $\rho(a, T)$ has a non-trivial measure and it is given by $\rho(a, T) = a^{(1-3\lambda)/2} |\Psi(a, T)|^2$. The continuity equation from equation (3.31) reads

$$\frac{\partial \rho}{\partial T} - \frac{\partial}{\partial a} \left[\frac{a^{3\lambda-1}}{2} \frac{\partial S}{\partial a} \rho \right] = 0, \quad (3.36)$$

which implies in the de Broglie-Bohm interpretation that

$$\frac{\partial a}{\partial T} = -\frac{a^{3\lambda-1}}{2} \frac{\partial S}{\partial a}, \quad (3.37)$$

in accordance with the classical relations $\dot{a} = \{a, H\} = -a^{3\lambda-1} P_a/2$ and $P_a = \partial S/\partial a$.

Inserting the phase from (3.35) into (3.37), we obtain the Bohmian quantum trajectory for the scale factor

$$a(T) = a_b \left[1 + \left(\frac{T}{T_b} \right)^2 \right]^{\frac{1}{3(1-\lambda)}}. \quad (3.38)$$

Note that this solution has no singularities and tends to the classical solution when $T \rightarrow \pm\infty$. Remember that we are in the gauge $N = a^{3\lambda}$, and T is related to conformal time through

$$N dT = a d\eta \Rightarrow d\eta = a(T)^{3\lambda-1} dT \quad (3.39)$$

Therefore, T_b is the characteristic time-scale of the bounce.

Note from (3.31) (with $\Psi = R e^{iS}$) that S satisfies the modified Hamilton–Jacobi equation,

$$\frac{\partial S}{\partial T} - \frac{a^{3\lambda-1}}{4} \left(\frac{\partial S}{\partial a} \right)^2 - Q = 0, \quad (3.40)$$

with the quantum potential given by

$$Q = -\frac{a^{(3\lambda-1)/2}}{4R} \frac{\partial}{\partial a} \left[a^{(3\lambda-1)/2} \frac{\partial R}{\partial a} \right]. \quad (3.41)$$

Hence, the trajectory (3.37) will not coincide with the classical trajectory whenever Q is comparable with the

other terms present in equation (3.40). In particular, the quantum potential justifies the bounce in solution (3.38) even when it is classically forbidden (for a radiation-dominated universe, for instance). In fact, using (3.41) together with (3.38), and extracting R from (3.35), it can be shown that the quantum potential assumes the simple form

$$\frac{1}{(T^2 + T_b^2)} \left[\frac{T_b}{2} - \frac{4 a_b^{3(1-\lambda)}}{9(1-\lambda)^2} \right], \quad (3.42)$$

which is stronger near the bounce. Moreover, the fact that the quantum potential vanishes at infinity is consistent with the universe becoming classical away from the bounce.

3.3.2 Radiation and Matter

A more elaborated and detailed model containing two fluids, dust and radiation, can be found in [69]. The model parameters can be chosen such that the radiation fluid dominates during the bounce, and the dust fluid dominates far from the bounce scale. The Bohmian trajectory for the scale factor coming from the phase of the wave solution of the corresponding Wheeler-DeWitt equation reads

$$a(\eta) = a_e \left[\left(\frac{\eta}{\eta_*} \right)^2 + 2 \frac{\eta_b}{\eta_*} \sqrt{1 + \left(\frac{\eta}{\eta_b} \right)^2} \right], \quad (3.43)$$

where a_e is the scale factor at matter-radiation equality, and the parameters η_* and η_b are related to the wavefunction parameters (similar to the case of a single fluid where the spread of the initial Gaussian distribution T_b ends up being the bouncing time scale).

It is, nonetheless, more convenient to reparametrize the bouncing trajectory with observable related quantities. In this section, all quantities calculated at a time when the scale factor has the same value as today will be denoted by the subscript $_0$. Expanding equation (3.43) for large η , we obtain the Hubble parameter

$$H^2 \approx \frac{4 a_e}{\eta_*^2} \left(\frac{1}{a^3} + \frac{a_e}{a^4} \right), \quad (3.44)$$

from where we can readily identify the dimensionless density parameters today $\Omega_{m0} = \rho_{m0}/\rho_{crit0}$ and $\Omega_{r0} = \rho_{r0}/\rho_{crit0}$ as the coefficients of $(a_0/a)^3$ and $(a_0/a)^4$, respectively

$$\Omega_{m0} = \frac{a_e}{a_0} \frac{4 R_H^2}{\eta_*^2}, \quad \Omega_{r0} = \left(\frac{a_e}{a_0} \right)^2 \frac{4 R_H^2}{\eta_*^2}, \quad (3.45)$$

where $\rho_{crit0} = 3H_0^2/(8\pi G)$ is the critical density today, $R_H = 1/(a_0 H_0)$ is the co-moving Hubble radius, ρ_{m0} and ρ_{r0} the energy densities of matter and radiation.

Next, expanding the Hubble parameter for large η_* , that is, considering the fluid near the bounce, we get

$$H^2 \approx H_0^2 \left(x^4 - \frac{\eta_b^2 x^6}{R_H^2} \right),$$

where we introduced the redshift-like variable $x = a_0/a$. From the expression above, we see that near the quantum bounce the Hubble parameter evolves as a classical Hubble parameter in the presence of a radiation fluid with density parameter Ω_{r0} , and a stiff matter fluid with negative density parameter given by

$$\Omega_{q0} = -\frac{\Omega_{r0}}{x_b^2}, \quad x_b = \frac{R_H}{\eta_b \sqrt{\Omega_{r0}}}. \quad (3.46)$$

Hence, the quantum effect we have calculated, which stops the contraction and realizes the bounce, is effectively equivalent to a bounce caused by the presence of an additional stiff matter fluid with negative energy, besides the usual matter and radiation fluids, in a classical cosmological scenario obeying the Friedmann equation. Note, however, that this equivalence is valid only at the background level. Using these new parameters, we obtain

$$H^2 \approx H_0^2 x^4 \left[1 - \left(\frac{x}{x_b} \right)^2 \right], \quad (3.47)$$

Consequently, x_b provides the scale factor where the bounce takes place (apart from a small correction coming from the dust matter density). Finally, we can invert the expressions above to obtain the wave-function parameters in terms of the observable related ones,

$$a_e = a_0 \frac{\Omega_{r0}}{\Omega_{m0}}, \quad \eta_* = 2R_H \frac{\sqrt{\Omega_{r0}}}{\Omega_{m0}}, \quad \eta_b = \frac{R_H}{x_b \sqrt{\Omega_{r0}}}. \quad (3.48)$$

The curvature scale at the bounce can be calculated as

$$L = \frac{1}{\sqrt{R}} \Big|_{\eta=0} = \sqrt{\frac{a^3(\eta)}{6 a''(\eta)}} \Big|_{\eta=0} = \frac{a_b \eta_b}{\sqrt{6(2\gamma_b + 1)}} = \frac{1}{\sqrt{(2\gamma_b + 1)}} \frac{a_0 R_H}{x_b^2 \sqrt{6 \Omega_{r0}}} \quad (3.49)$$

where R is the four dimensional Ricci scalar and

$$\gamma_b = \frac{\Omega_{m0}}{(4 x_b \Omega_{r0})} \quad (3.50)$$

is the ratio of the dust and radiation matter density at the bounce (where the factor of 4 was included for later convenience). Imposing that the bounce scale is larger than the Planck scale, $L_b > L_p$, we can obtain an upper bound on x_b . This bound is relevant since we expect that the Wheeler–DeWitt equation should be a valid approximation for any fundamental quantum gravity theory at scales smaller than the Planck length. Using

$H_0 = 70 \text{ Km s}^{-1} \text{ Mpc}^{-1}$ we obtain

$$\frac{a_0 R_H}{L_p} \approx 8 \times 10^{60}, \quad (3.51)$$

and consequently,

$$x_b \lesssim \frac{\sqrt{8}}{(6\Omega_{r0})^{1/4}} \times 10^{30} \approx 2 \times 10^{31}. \quad (3.52)$$

In the above calculation, we assumed $\gamma_b \ll 1$ because the bounce must also happen at energy scales higher than the start of the nucleosynthesis (around 10 MeV), which implies $x_b \gg 10^{11}$ (using cosmic microwave background radiation temperature $T_{\gamma 0} \approx 2.7 \text{ K}$), and we are assuming that Ω_{r0} should not be much smaller than its usual value $\Omega_{r0} \approx 8 \times 10^{-5}$. Hence we get

$$10^{11} \ll x_b < 10^{31}. \quad (3.53)$$

Next, using the parameters above, we define

$$\bar{\eta} = \frac{\eta}{\eta_b}, \quad \bar{k} = k \eta_b, \quad r_b = m a_b \eta_b, \quad (3.54)$$

which are the natural parameters appearing in the equations we will solve, as we will see in the following sections (m here is the mass of the scalar field whose particles are created at the bounce). With this definition, it is easy to see that

$$r_b = \frac{a_b \eta_b}{L_c} \approx \frac{L_b}{L_c}, \quad L_c = \frac{1}{m}, \quad (3.55)$$

where L_c is the Compton wavelength of the massive particle. Note that usually $r_b \ll 1$ because the curvature scale at the bounce is much smaller than the Compton wavelength, or the mass of the particle is much smaller than the mass–energy scale at the bounce.

In terms of the new parameters, the Bohmian trajectory reads (compare it with (2.9) and (2.11))

$$a(\eta) = a_b \left(\bar{\eta}^2 \gamma_b + \sqrt{1 + \bar{\eta}^2} \right) \quad (3.56)$$

Note that, the dust and radiation terms have equal weight at $\bar{\eta}_e \approx 1/\gamma_b$, which is the same result one would obtain substituting a_e in the equation above. In the case of pure radiation ($\Omega_{m0} = 0$ and, therefore, $\gamma_b = 0$), the scale factor reduces to

$$a(\eta) = a_b \sqrt{1 + \bar{\eta}^2}, \quad (3.57)$$

which is exactly the trajectory given in equation (3.38) for a radiation fluid ($\lambda = 1/3$).

Chapter 4

Gravitational Particle Creation in de Broglie–Bohm Quantum Bouncing Models

... then you'll see that it is not the spoon that bends, it is only yourself.

The Matrix.

In this chapter, we finally calculate the Bogoliubov coefficients of scalar particle creation in the two bouncing models derived in the last chapter. However, we first give a lightspeed review of quantization in a curved spacetime. More details can be found, for instance, in [70–75]. Only the very basics though is necessary for the calculation of the Bogoliubov coefficients.

4.1 Scalar Field in Curved Space-Time

In a curved space-time, the generalization of the action of a scalar field φ reads

$$S = \frac{1}{2} \int d^4x \sqrt{-g} \left[g^{\mu\nu} \varphi_{,\mu} \varphi_{,\nu} - (m^2 + \xi R) \varphi^2 \right] \quad (4.1)$$

where $g = |\det g^{\mu\nu}|$, R is the curvature Ricci scalar and ξ is a dimensionless number taken as free parameter just as m , the mass of the field. ξ is called the coupling term between the scalar field and gravity. The Klein-Gordon equation from the above action reads

$$\left(\square + m^2 + \xi R \right) \varphi = 0 \quad \text{or} \quad \frac{1}{\sqrt{g}} \left(\sqrt{g} g^{\mu\nu} \varphi_{,\mu} \right)_{,\nu} + (m^2 + \xi R) \varphi = 0. \quad (4.2)$$

where the second form is more convenient for an actual calculation. It looks like ξ induces a mass correction proportional to the curvature scalar (see, however, [76]). The case $\xi = 0$ is called minimal coupling. Another particularly interesting case is

$$\xi = \frac{n-2}{4(n-1)} \quad (4.3)$$

where n is the space-time dimension. This is called conformal coupling, because the Klein-Gordon equation becomes invariant with respect to conformal transformations when $m = 0$ [39, 71]. A conformal transformation is a transformation of the form $g_{\mu\nu}(x) \rightarrow \bar{g}_{\mu\nu}(x) = \Omega^2(x) g_{\mu\nu}$, where Ω is a real, continuous but otherwise arbitrary function. In 2-dimensional models there is no difference between minimal and conformal coupling. The conformal symmetry simplifies the field equations in a conformally flat space-time, where $g_{\mu\nu}(x) = \Omega^2(x) \eta_{\mu\nu}$, as in the flat FLRW universe.

As in Minkowski space-time, the solutions to the Klein-Gordon equation in a curved space-time define a scalar product

$$(u, v) = -i \int d\Sigma^\mu \sqrt{\bar{g}_\Sigma} \left(u \overleftrightarrow{\partial}_\mu v^* \right) = -i \int d\Sigma^\mu \sqrt{\bar{g}_\Sigma} \left(u v_{,\mu}^* - u_{,\mu} v^* \right) \quad (4.4)$$

where $d\Sigma^\mu = \eta^\mu d\Sigma$, $d\Sigma$ is the volume element in a space-like surface Σ , η^μ is a future directed normalized vector orthogonal to Σ , and \bar{g}_Σ is the determinant of the space part of the metric in Σ . The product of two solutions is conserved, it does not depend on Σ ,

$$(u, v)_{\Sigma_1} = (u, v)_{\Sigma_2}. \quad (4.5)$$

The proof is as follows. Consider two solutions u and v that vanish at spatial infinity (if space is compact, one

can impose time-like conditions such that $u = v = 0$), and V the volume limited by Σ_1 and Σ_2 . We have

$$(u, v)_{\Sigma_1} - (u, v)_{\Sigma_2} = -i \oint_{\partial V} d\Sigma^\mu \sqrt{g_\Sigma} \left(u \overleftrightarrow{\partial}_\mu v^* \right) = -i \int_V dV g^{\mu\nu} \left(u \overleftrightarrow{\partial}_\mu v^* \right)_{;\nu} = 0, \quad (4.6)$$

where the Gauss law has been used and the last equality follows since u and v are both solutions to the Klein-Gordon equation, so the integrand vanishes.

4.2 Bogoliubov Coefficients

The quantization of a theory in a curved space–time follows analogously the formalism in Minkowsky space: the equations of motion are postulated together with the operator algebra, the Fock space is constructed, then the physical states and the observables are interpreted.

From the action (4.1) it follows that the momentum canonically conjugate to $\varphi(x)$ reads

$$\pi(x) = \frac{\partial \mathcal{L}}{\partial(\varphi,0)} = \sqrt{g} g^{0\mu} \varphi,_{\mu} \quad (4.7)$$

and the operator algebra reads

$$\left[\varphi(x^0, x^i), \varphi(x^0, x'^i) \right]_{\Sigma} = \left[\pi(x^0, x^i), \pi(x^0, x'^i) \right]_{\Sigma} = 0, \quad (4.8)$$

$$\left[\varphi(x^0, x^i), \pi(x^0, x'^i) \right]_{\Sigma} = i \delta^{n-1}(x^i - x'^i), \quad (4.9)$$

where $\int d\Sigma \delta^{n-1}(x^i - x'^i) = 1$. The commutation relations do not depend on the chosen space–like surface Σ .

The construction of the Fock space follows as in Minkowski space–time.

There is, however, an ambiguity in the choice of a particular representation. The commutation relations define the canonical variables for a particular problem: they are algebraic relations that do not depend on the Hamiltonian, that is the dynamics. These variables completely define the system at each moment so that any physical quantity can be expressed in terms of them. However, to determine the dynamical evolution it is necessary to represent the variables as operators in a Hilbert space subject to the Heisenberg equations.

In non–relativistic quantum mechanics, that is, in systems with finitely many degrees of freedom, the choice of the representation is irrelevant since the irreducible representations of the canonical commutation relations are unitarily equivalent. This is the Von Neumann theorem. The choice of a particular representation reduces to a matter of convenience.

In systems with infinitely many degrees of freedom, as in quantum field theory, the Von Neumann theorem does not apply and the choice of a particular representation of the field operators algebra may have a physical meaning due to the existence of inequivalent representations.

The Bogoliubov transformations are linear transformations between the expansion bases of a field operator such the the canonical commutation relations are preserved. They are thus also called canonical transformations. The calculation of the Bogoliubov coefficients is a way of verifying the equivalence of two representations, in particular, of vacuum states relative to two different observers.

Let there be two complete orthonormal bases of solutions, $\{u_i(x), u_i^*(x)\}$ and $\{v_j(x), v_j^*(x)\}$, such that the

field $\varphi(x)$ can be expanded in one or another basis,

$$\varphi(x) = \sum_i \left[a_i u_i(x) + a_i^\dagger u_i^*(x) \right] = \sum_j \left[b_j v_j(x) + b_j^\dagger v_j^*(x) \right]. \quad (4.10)$$

In general, each decomposition defines a different vacuum state, $|0_u\rangle$ and $|0_v\rangle$, that is

$$a_i |0_u\rangle = 0, \quad \forall i \quad (4.11)$$

$$b_j |0_v\rangle = 0, \quad \forall j$$

and, in general,

$$a_i |0_v\rangle \neq 0, \quad (4.12)$$

$$b_j |0_u\rangle \neq 0.$$

There are thus two distinct Fock states. Since both sets are complete, the modes $\{v_j(x), v_j^*(x)\}$ can be written as linear combinations of the modes $\{u_i(x), u_i^*(x)\}$

$$v_j(x) = \sum_i \left[\alpha_{ji} u_i(x) + \beta_{ji} u_i^*(x) \right], \quad \text{and, inversely} \quad u_i(x) = \sum_j \left[\alpha_{ji}^* v_j(x) - \beta_{ji} v_j^*(x) \right]. \quad (4.13)$$

These are the Bogoliubov transformations and the α_{ij} and β_{ij} are the Bogoliubov coefficients. Since the bases are orthonormal, the Bogoliubov coefficients can be calculated as internal products between the modes,

$$\alpha_{ij} = (v_i, u_j), \quad (4.14)$$

$$\beta_{ij} = -(v_i, u_j^*).$$

The Bogoliubov coefficients have the following properties

$$\sum_k \left(\alpha_{ik} \alpha_{jk}^* - \beta_{ik} \beta_{jk}^* \right) = \delta_{ij}, \quad (4.15)$$

$$\sum_k \left(\alpha_{ik} \beta_{jk} - \beta_{ik} \alpha_{jk} \right) = 0.$$

With these coefficients, the operators a_i and a_i^\dagger can be written as linear combinations of b_j and b_j^\dagger

$$\begin{aligned} \sum_i [a_i u_i(x) + a_i^\dagger u_i^*(x)] &= \sum_j [b_j v_j(x) + b_j^\dagger v_j^*(x)] \\ &= \sum_j \left\{ b_j \sum_i [\alpha_{ji} u_i(x) + \beta_{ji} u_i^*(x)] + b_j^\dagger \sum_i [\alpha_{ji}^* u_i^*(x) + \beta_{ji}^* u_i(x)] \right\} \\ &= \sum_{i,j} \left[(\alpha_{ji} b_j + \beta_{ji}^* b_j^\dagger) u_i(x) + (\beta_{ji} b_j + \alpha_{ji}^* b_j^\dagger) u_i^*(x) \right] \end{aligned} \quad (4.16)$$

such that

$$a_i = \sum_j (\alpha_{ji} b_j + \beta_{ji}^* b_j^\dagger), \quad \text{and, similarly,} \quad b_j = \sum_i (\alpha_{ji}^* a_i - \beta_{ji}^* a_i^\dagger). \quad (4.17)$$

It follows immediately that Fock spaces are not equivalent if $\beta_{ij} \neq 0$. In particular, the vacuum state associated to the modes $\{u_i(x), u_i^*(x)\}$ does not correspond to the vacuum state associated to $\{v_j(x), v_j^*(x)\}$

$$a_i |0_v\rangle = \sum_j \beta_{ji}^* b_j^\dagger |0_v\rangle \neq 0 \quad (4.18)$$

The expectation value of the number operator of the particles associated to the modes $\{u_i(x), u_i^*(x)\}$, $N_i = a_i^\dagger a_i$, in the state $|0_v\rangle$ is

$$\langle 0_v | N_i | 0_v \rangle = \sum_j |\beta_{ji}|^2, \quad (4.19)$$

which means that the vacuum associated to the modes $\{v_j(x), v_j^*(x)\}$ contains $\sum_j |\beta_{ji}|^2$ particles associated to the modes $\{u_i(x), u_i^*(x)\}$. From equation (4.13), if any one of the β_{ji} is nonzero, v_j contains a mixture of positive and negative frequency modes, $u_i(x)$ and $u_i^*(x)$, and the observer associated to the base $\{v_j(x), v_j^*(x)\}$ will detect particles where there is just vacuum for the observer associated to $\{u_i(x), u_i^*(x)\}$. Only when all the β_{ji} are zero, the states $|0_u\rangle$ and $|0_v\rangle$ are equivalent. In that case, $b_i |0_u\rangle$ and $a_j |0_v\rangle$, so that both representations share the same vacuum state.

The field must be decomposed into positive and negative frequency components before the creation and annihilation operators are defined. This decomposition is different for inequivalent observers, although they are related by a Bogoliubov transformation. This explains why the number of particles, defined in terms of creation and annihilation operators, are different in one or another representation. In Minkowski space-time, the Poincaré group allows a natural choice: the modes $u_k(x)$ associated with the Lorentz observers that are eigenfunctions of the Killing vectors $\partial/\partial t$ orthogonal to the surfaces $t = \text{constant}$. Since the vacuum state is invariant with respect to the Poincaré group, the Lorentz observers form an equivalence class. In a curved space-time, however, the Poincaré group is no longer a symmetry group. In general, there are no Killing vectors to define positive frequency modes, and even when there is a symmetry that allows us to define these modes, the

principle of general covariance does not allow us to consider a particular coordinate system. Coordinate systems are physically irrelevant. Consequently, the concept of particles is ambiguous, and the physical interpretation of quantum states is more subtle.

The concept of particles was originally introduced with respect to inertial observers and it was assumed to be independent of the state of motion of the observer. However, the concept of vacuum, and therefore the concept of particles, depends on the field operators algebra representation and, in particular, on the state of motion of the observer and on the geometry of space–time. The ambiguity in the concept of particles may seem counterintuitive at first sight. However, by the Heisenberg uncertainty principle, the concept of vacuum is not the same as empty space, since all space is filled by the fields that make up all the matter in the universe. The vacuum state is simply the state of least possible energy of these fields. The energy states are defined by the Hamiltonian operator based on local conditions in space–time. Since each observer amounts to one equivalence class of coordinate systems, they observe different quantum states and, in particular, distinct vacuum states.

4.3 Gravitational Particle Creation in Bouncing Models

The Klein–Gordon equation for the modes of a free massive scalar field φ in a flat FLRW background reads

$$\frac{\partial^2 \phi_k}{\partial \eta^2} + \left[k^2 + m^2 a^2 - (1 - 6\xi) \frac{a''}{a} \right] \phi_k = 0, \quad (4.20)$$

where $\phi_k = a \varphi_k$. Using the scale factor from equation (3.56) and the parameters (3.54), the mode equation reads

$$\phi_k'' + (\nu^2 - V) \phi_k = 0, \quad (4.21)$$

where

$$V = (1 - 6\xi) \frac{\left[(1 + \bar{\eta}^2)^{-3/2} + 2\gamma_b \right]}{(1 + \bar{\eta}^2)^{1/2} + \bar{\eta}^2 \gamma_b}, \quad (4.22)$$

$$\nu^2 = \bar{k}^2 + \frac{r_b^2 a^2}{a_b^2}. \quad (4.23)$$

V is the gravitational potential felt by the modes ϕ_k , and ν the frequency of the mode k . It should be noted that, in the presence of the dust fluid, the potential decays slower away from the bounce, see figure 4.1.

Given a complete set of solutions for the mode equation (4.21), a set of creation and annihilation operators is defined, and consequently a vacuum state [71, 77]. The ambiguity in defining the vacuum state stems from the fact that we do not have a general procedure to define a unique set of modes when space–time does not possess a global time-like Killing vector. One special and suitable choice is the so called adiabatic vacuum [71, 72, 75]. One of the main physical properties of this vacuum state choice is that its vacuum expectation value of the number operator varies minimally when the expansion rate of the universe becomes arbitrarily slow (see also [77] for a good review on that). As discussed in [77], for a given mode k at a time η , the adiabatic vacuum can be defined up to a maximum order $N_{k,\eta}$.¹ The maximum order $N_{k,\eta}$ is a monotonically increasing function of k . Therefore, large k 's have less ambiguity in their vacuum definition than small k 's.

The adiabatic vacuum state has two points relevant to our problem. First, it may depend on the time chosen to define it. If we impose the adiabatic vacuum condition at a time η_i and evolve the modes through equation (4.21) until η_f , we may obtain a different set of mode functions we would otherwise get by imposing the adiabatic vacuum condition at η_f . The other point about this procedure, which is a consequence of the existence of the maximum adiabatic order $N_{k,\eta}$ discussed above, is that it cannot be applied for all modes k , as it depends on the behavior of the mode functions, and for a given time η only a subset of modes behave in an

¹ This is a consequence of the fact that the adiabatic expansion is asymptotic. However, in some special cases the series is convergent, and the vacuum can be defined up to an arbitrary function that decreases faster than any finite power of k^{-1} .

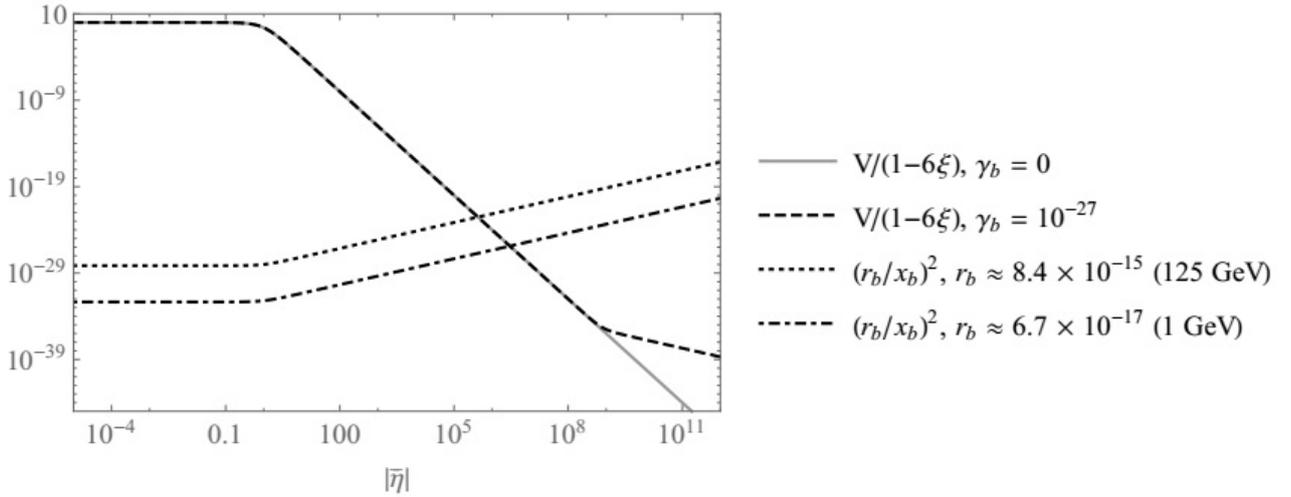


Figure 4.1: This shows the gravitational potential $V = a''/a$ and the mass term $m^2 a^2$ in equation (4.21). In the initial phase, the potential V grows as a power law. If there is dust, then the power-law changes during the dust radiation transition. The potential attains its maximum near the bounce. In the minimally coupled case ($\xi = 0$), the maximum of the potential is $V \approx 1$. These features of the potential V are shown in the continuum and dashed lines. In the massive case, the mass term dominates the mode evolution at early times and the larger the mass, the longer it dominates. This is shown by the dotted and dot-dashed lines in the figure. Note that the mass term dominates the gravitational potential V up to the radiation dominated epoch, unless the particle mass is very small ($m < 10$ eV). Hence the presence of dust does not affect much the particle production. For the same reason, the solutions at past and future infinity do not depend on ξ .

adiabatic manner.²

The first point can be laid down as follows: given a mode k at η_i , we impose that the mode initial conditions for ϕ_k are given by the adiabatic approximation up to the maximum order N_{k,η_i} . Using this as the initial condition in (4.21), we obtain the solution $\phi_k^{(i)}(\eta)$. Repeating the process at a time η_f and comparing both solutions at η_f , we have

$$\phi_k^{(i)}(\eta_f) - \phi_k^{(f)}(\eta_f) \lesssim \mathcal{O}\left(k^{-N_{k,[\eta_i, \eta_f]}}\right), \quad (4.24)$$

where $N_{k,[\eta_i, \eta_f]}$ is the maximum adiabatic order attainable in the interval $[\eta_i, \eta_f]$.³ To measure the difference between vacua, we introduce the norm squared of the Bogoliubov coefficients given by [71, 75]

$$\left|\beta_k^{(i,f)}\right|^2 = \left|\phi_k^{(i)} \phi_k^{(f)'} - \phi_k^{(f)} \phi_k^{(i)'}\right|^2 = n_k^{(i,f)}, \quad (4.25)$$

The quantity $n_k^{(i,f)}$ is the number density of particles with mode k measured by observers in the adiabatic vacuum defined at η_f if the initial state was the adiabatic vacuum defined at η_i .

Suppose that the adiabatic approximation is valid through the whole interval $[\eta_i, \eta_f]$. It means that there is

²Alternatively, one can impose a vacuum state by choosing a boundary condition. This asymptotic state is sometimes called "Bunch-Davies vacuum". Nonetheless, this choice is not free from ambiguities, and coincides with the adiabatic vacuum up to its approximation order [77].

³See, for example, eq. (33) of [77].

some $N_{k, [\eta_i, \eta_f]} > 0$, and consequently

$$n_k^{(i,f)} \lesssim \mathcal{O}\left(k^{-N_{k, [\eta_i, \eta_f]}}\right). \quad (4.26)$$

In other words, in the ultraviolet limit ($k \rightarrow \infty$), the \bar{k}^2 frequency present in (4.21) dominates over all other terms. Also, it can be shown that the maximum adiabatic order $N_{k, \eta}$ increases to infinity in this limit. This is equivalent to say that in the ultraviolet limit there is a strong suppression in the number of particles created: as the adiabatic order goes to infinity, any ambiguity in the vacuum definition must fall faster than any finite power of k^{-1} , as an exponential decay. Hence, there is no divergence in the UV limit, and the particle production is finite (unless some infrared divergence is present).

Inspecting figure 4.1, we note that the potential V has a maximum at the bounce. Therefore, any mode with $\bar{k}^2 \gg V(\eta = 0)$ will be in the adiabatic regime during its whole evolution, including through the bounce itself, and hence particle production of such modes will be exponentially suppressed. This was verified numerically, as we will see. The maximum of the potential thus provides a natural cutoff. On the other hand, for $\bar{k}^2 \lesssim V(\eta = 0)$ there is a time interval where the adiabatic approximation fails, and particle creation takes place.

An important comment has to be made now: in [78], all calculations are done for modes much less than the Hubble radius at all epochs of their cosmological scenario, which is physically the ultraviolet limit ($\bar{k}^2 \gg V$). Hence, as we discussed above, there is an exponential cutoff for these modes, and particle production is heavily suppressed. Another way to phrase it can be: for modes which never cross the potential, the adiabatic vacuum solution, which matches the boundary condition in the far past before the bounce, is always a good approximation at any time. Hence, it coincides with the solution obtained through the adiabatic boundary condition prescribed in the far future after the bounce. Consequently, one must have $\beta_k \approx 0$ for these modes. The particle production which is obtained in [78] comes from the matching conditions they impose, which does not capture the precise quantitative evolution of mode function for these large k modes. In other words, they artificially introduce a background discontinuity through the matching approximation. Note that, in [79], a discontinuity in the background between the different phases is assumed from the beginning, and this gives rise to particle production which depends explicitly on the assumed discontinuity. In practice, the discontinuity creates an infinite potential, invalidating the adiabatic approximation at that point.

As for the second point, we want to calculate the amount of particle creation using the above adiabatic vacuum prescription for all modes k . Thus, if the adiabatic vacua are defined at $\bar{\eta}_i \rightarrow -\infty$ and $\bar{\eta}_f \rightarrow \infty$, the first order adiabatic vacuum state, given by the zeroth order WKB solutions of equation (4.21), coincides with the infinite order adiabatic vacua, and hence they precisely define state solutions for all modes k . In practice, we will consider that the scalar field is initially in the adiabatic vacuum state in the far past ($\bar{\eta}_i \ll 1$), compute the evolution of such modes until the expansion era far from the bounce ($\bar{\eta}_f \gg 1$), and compare it to the adiabatic vacuum at $\bar{\eta}_f$. That is why we numerically prescribe our initial conditions far from the bounce, in the past and

in the future, through first order adiabatic approximated solutions, and we verify that the initial approximations coincide with the numerical solutions obtained with such boundary conditions for a long interval of time $\bar{\eta}$ before the adiabatic approximation loses its validity.

We are also interested in the energy density of the created particles. Using a vacuum definition at $\bar{\eta}_i$ as our system state, the expectation value of the energy density at any time $\bar{\eta}$ with respect to this vacuum is

$$\langle \rho \rangle_{(i)} = \frac{1}{a^4 \eta_b} \int \frac{d^3 k}{(2\pi)^3} \frac{1}{2} \left[\left| \phi_k^{(i)'} \right|^2 + \left(\nu^2 + \mathcal{H}^2 \right) \left| \phi_k^{(i)} \right|^2 - \mathcal{H} \left(\phi_k^{(i)*} \phi_k^{(i)} \right)' \right], \quad (4.27)$$

where $\mathcal{H} = a'/a$.

As it is well known, the energy density of a scalar field in curved space time is divergent. Not only the usual divergence obtained in Minkowsky but new ones must be taken care of. Nonetheless, in this work we want to study the amount of energy resulting from particle creation in bouncing models. For this reason we introduce the expected value of the energy density for the adiabatic vacuum defined at $+\infty$, that is, $\langle \rho \rangle_{(f)}$. Then, the difference of the average energy density of scalar particles evaluated in the far past adiabatic vacuum state and in the far future adiabatic vacuum state,

$$\Delta \rho = \langle \rho \rangle_{(i)} - \langle \rho \rangle_{(f)}, \quad (4.28)$$

yields a finite quantity (see [71]), which represents the amount of energy of scalar particles created between the far past and the far future of a bouncing model as seen from the point of view of observers in the far future, with their appropriate choice of adiabatic vacuum state. As we will see, this production is effective mainly in the bouncing phase itself. We can relate the mode functions associated to both states as

$$\phi_k^{(f)}(\bar{\eta}) = \alpha_k^{(i,f)} \phi_k^{(i)}(\bar{\eta}) + \beta_k^{(i,f)} \phi_k^{(i)*}(\bar{\eta}). \quad (4.29)$$

The Bogoliubov coefficients $\beta_k^{(i,f)}$ can be readily calculated using (4.25). In the far future, when the modes $\phi_k^{(f)}$ are deep in the adiabatic phase, the energy difference is given by

$$\Delta \rho = \frac{1}{2 \pi^2 \eta_b^4 a^4} \int_0^\infty d\bar{k} \bar{k}^2 n_k^{(i,f)} \nu, \quad (4.30)$$

and the number density of created particles is

$$n = \frac{1}{2 \pi^2 \eta_b^3 a^3} \int_0^\infty d\bar{k} \bar{k}^2 n_k^{(i,f)}. \quad (4.31)$$

In the massive case, this provides the energy density when a is large enough and consequently $\nu \approx a r_b$ for modes

relevant to the integral above, that is, when modes satisfying $\bar{k} \ll a r_b/a_b$ are dominant for the integral. As we will see below, the particle number density $n_k^{(i,f)}$ has an exponential cutoff in the ultraviolet limit, therefore, for the massive case and a large enough, we have

$$\Delta\rho \approx m n, \quad (4.32)$$

In the massless case, $m = 0$, where the frequency term is $\nu = \bar{k}$, the energy density yields the usual result for a relativistic fluid,

$$\Delta\rho = \frac{1}{2\pi^2 \eta_b^4 a^4} \int_0^\infty d\bar{k} \bar{k}^3 n_k^{(i,f)}. \quad (4.33)$$

4.3.1 Bouncing with a Radiation Fluid

In this section, we consider a Bohmian solution of the Wheeler–DeWitt equation obtained in [80] for the case of a universe dominated by a radiation perfect fluid only. In this case, the scale factor is described by equation (3.57). The Klein–Gordon equation (4.21) simplifies to

$$\phi_k'' + \left[\bar{k}^2 + r_b^2 (1 + \bar{\eta}^2) - \frac{(1 - 6\xi)}{(1 + \bar{\eta}^2)^2} \right] \phi_k = 0. \quad (4.34)$$

Note that the ξ dependent term in (4.34) goes to zero at both past and future infinity, $\bar{\eta} \rightarrow \pm\infty$, for whatever value of ξ . Therefore, the vacuum solutions at these asymptotic limits do not depend on ξ . Figure 4.1 shows the gravitational potential and the mass term for a few different cases. The potential goes to zero whether there is dust or not, but it goes to zero slower if there is. In the massless case, the total modification to the frequency vanishes asymptotically, giving simple plane–waves as asymptotic solutions of (4.34) for any value of ξ . In the massive case, the mass term dominates for $|\bar{\eta}| \gg 1$, while the ξ dependent term vanishes in this limit. Hence, the asymptotic solutions are mass dependent, but still do not depend on ξ .

Radiation Fluid with Conformal Coupling

Let us start with the simple conformally coupled case ($\xi = 1/6$), which is well–known in the literature [71, 81, 82]. The time dependency of the frequency is determined by the mass term alone, shown in figure 4.1, and equation (4.34) reduces to

$$\phi_k'' + \left[\bar{k}^2 + r_b^2 (1 + \bar{\eta}^2) \right] \phi_k = 0. \quad (4.35)$$

This has exact solutions in terms of parabolic cylinder functions [83]. The normalized solutions that match the adiabatic vacuum solution are [71]

$$\phi_k^{(i)}(\bar{\eta}) = (2r_b)^{-1/4} \exp\left(-\frac{\pi}{8}\lambda\right) D_{i\frac{\lambda-1}{2}}\left[(i-1)\sqrt{r_b}\bar{\eta}\right], \quad \bar{\eta} < 0 \quad (4.36)$$

$$\phi_k^{(f)}(\bar{\eta}) = \phi_k^{(i)*}(-\bar{\eta}), \quad \bar{\eta} > 0 \quad (4.37)$$

where

$$\lambda = r_b \left(1 + \frac{\bar{k}^2}{r_b^2}\right). \quad (4.38)$$

To calculate the Bogoliubov coefficients, we use the identity [83]

$$D_\nu(z) = e^{i\pi\nu} D_\nu(-z) + \frac{\sqrt{2\pi}}{\Gamma(-\nu)} e^{i\frac{\pi}{2}(\nu+1)} D_{-\nu-1}(-iz) \quad (4.39)$$

to show that

$$\phi_k^{(i)}(\bar{\eta}) = \frac{\sqrt{2\pi} e^{i\pi/4}}{\Gamma\left(\frac{1-i\lambda}{2}\right)} \phi_k^{(f)}(\bar{\eta}) - i e^{-\pi\lambda/2} \phi_k^{(f)*}(\bar{\eta}) \quad (4.40)$$

It follows that

$$n_k^{(i,f)} = e^{-\pi\lambda} = \exp\left[-\pi r_b \left(1 + \frac{\bar{k}^2}{r_b^2}\right)\right], \quad (4.41)$$

which falls off faster than any inverse finite power of k or m . As it was explained in [81], this is the spectrum of a non-relativistic thermal gas of particles.

From equation (4.41), the number density of created particles is

$$n = \frac{1}{2\pi^2 \eta_b^3 a^3} \int d\bar{k} \bar{k}^2 n_k^{(i,f)} = \left(\frac{\sqrt{r_b}}{2\eta_b a}\right)^3 e^{-\pi r_b} = \left(\frac{\sqrt{\Omega_{r0}}}{a_0 R_H L_c}\right)^{3/2} \frac{x^3}{8} e^{-\pi r_b}. \quad (4.42)$$

The quantity $r_b = a_b \eta_b / L_c \approx L_b / L_c$ is usually very small. For instance, assuming $x_b = 10^{30}$ (which gives roughly $L_b \approx 10^3 L_p$) and the Higgs particle, one of the most massive scalar particles in the standard model, one gets $r_b = 8.4 \times 10^{-15}$. Hence, we can neglect the exponential in equation (4.42) due to the smallness of r_b . In other words, the exponential provides a very large mass cutoff

$$m_c = 4.7 \left(\frac{x_b}{10^{30}}\right)^2 \times 10^{15} \text{ GeV}. \quad (4.43)$$

Using equation (4.32), one can write the energy density of created particles for very large scale factors as

$$\Delta\rho = m n \approx m \left[\frac{x \Omega_r^{1/4}}{2(R_H L_c)^{1/2}}\right]^3 \approx \left(\frac{m}{m_H}\right)^{5/2} x^3 \times 10^{-44} \text{ g/cm}^3, \quad (4.44)$$

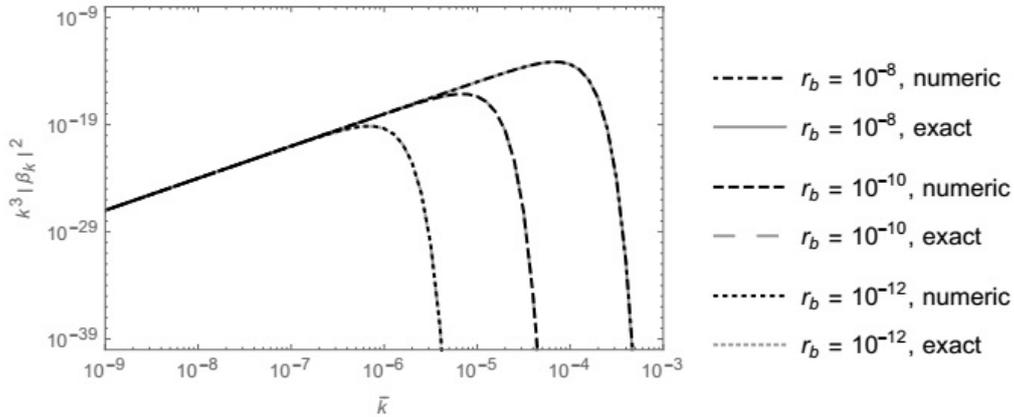


Figure 4.2: The Bogoliubov coefficients in the conformal coupling case for a few values of r_b . Our numerical solutions are compared with the exact solutions (4.41). See also [4].

where m_H is the Higgs mass (125 GeV), yielding

$$\Omega_\phi = \frac{\Delta\rho}{\rho_{crit0}} \approx \left(\frac{m}{m_H}\right)^{5/2} x^3 \times 10^{-15}. \quad (4.45)$$

In order to test our algorithm, we have also calculated equation (4.41) numerically. Later, we will follow analogous steps to calculate the Bogoliubov coefficients for the minimal coupling case. We have used equation (4.25), where $\phi_k^{(f)}$ is given in (4.37), and we used (4.36) and its derivative as the initial conditions to numerically evolve ϕ through (4.35) from an initial time $\bar{\eta}_i$ before the bounce to a final time $\bar{\eta}_f$ after the bounce. Since the solutions (4.36) and (4.37) are exact, we can choose any $\bar{\eta}_i$ and $\bar{\eta}_f$. However, we want to use the same algorithm in the minimal coupling case (with minor modifications). Therefore, we use as initial time $\bar{\eta}_i$ such that

$$\bar{k}^2 + r_b^2 (1 + \bar{\eta}_i^2) = 10^6 \times \frac{1}{(1 + \bar{\eta}_i^2)^2} \quad (4.46)$$

and, for convenience, $\bar{\eta}_f = -\bar{\eta}_i$. Note that the time of integration from $\bar{\eta}_i$ to $\bar{\eta}_f$ is greater for smaller values of k and r_b . The results are shown in figure 4.2.

Radiation Fluid with Minimal Coupling

Next, we calculate numerically the Bogoliubov coefficients for equation (4.34) in the minimal coupling case, $\xi = 0$, the generalization for any constant value of ξ being simple enough. As it can be seen from equation (4.34), the solutions do not depend on ξ at a sufficient time distance from the bounce, $|\bar{\eta}| \gg 1$. However, in this case, we have to distinguish the massive case from the massless case: the massless case is trivial only in the conformal coupling case, where equation (4.34) reduces to a collection of free harmonic oscillators and there is no particle

production.

Massless Case

In the massless minimally coupled case, the equation (4.34) for the modes reduces to

$$\phi_k'' + \left[\bar{k}^2 - \frac{1}{(1 + \bar{\eta}^2)^2} \right] \phi_k = 0, \quad (4.47)$$

It can be seen from the equation above that the minimal coupling term goes to zero at infinity, and the equation reduces to that of a simple harmonic oscillator. The vacuum mode solution is then given by

$$\phi_k(\bar{\eta}) = (2\bar{k})^{-1/2} \exp(-i\bar{k}\bar{\eta}). \quad (4.48)$$

In practice, from (4.47), the plane-wave vacuum solutions can be consistently used for $\bar{k} \gg 1/(1 + \bar{\eta}^2)$. Note that the maximum of the potential

$$V = \frac{1}{(1 + \bar{\eta}^2)^2} \quad (4.49)$$

is at the bounce, $\bar{\eta} = 0$. Any $\bar{k} < 1$ will therefore result in particle creation: there is an interval where the adiabatic approximation no longer holds. On the other hand, the modes $\bar{k} > 1$ are adiabatic during the whole evolution, and particle production is suppressed. Therefore, we expect an exponential cutoff at $\bar{k} \gtrsim 1$. These assertions are verified numerically.

To calculate the Bogoliubov coefficients, we follow the same algorithm as in the conformally coupled case, but with (4.48) to determine the initial conditions at $\bar{\eta}_i$ given by (4.46) (with $r_b = 0$). Our results are shown in figure 4.3 together with the massive case explained below. Integrating numerically in \bar{k} , we obtain the particle number density

$$n \approx \frac{6.7 \times 10^{-2}}{a^3 \eta_b^3} \approx 3 \times 10^{-2} x^3 \left(\frac{x_b}{10^{30}} \right)^3 \text{ cm}^{-3}. \quad (4.50)$$

We obtained this same result for massive particles, within the numerical precision, as we describe later. For massless particles, the energy density calculated through equation (4.33) gives

$$\Delta\rho \approx \frac{3 \times 10^{-2}}{a^4 \eta_b^4}, \quad \Omega_\phi = 2.5 \times 10^{-10} x^4 \left(\frac{x_b}{10^{30}} \right)^4. \quad (4.51)$$

Hence, only for $x_b > 10^{31}$ one should have a significant amount of massless scalar particles, which could exceed the radiation density in the universe. Note, however, that such x_b would imply $a_b \eta_b > L_p$, which goes beyond the scope of our calculations.

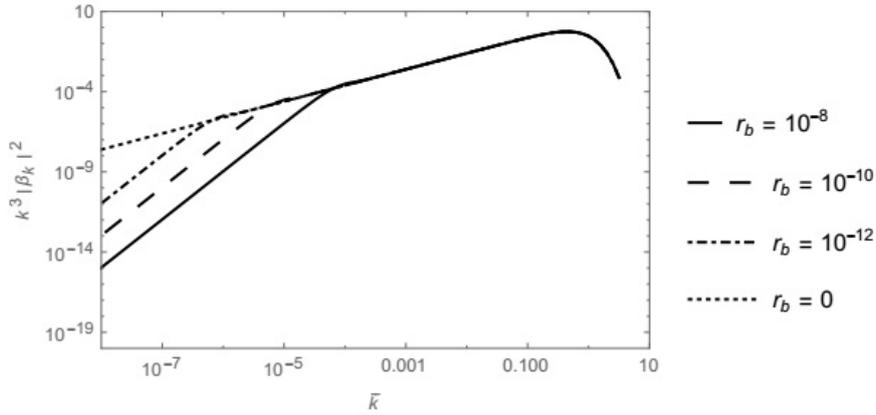


Figure 4.3: The Bogoliubov coefficients in the minimal coupling case for a few values of r_b . See also [4]. It can be seen that particle creation takes place mostly for \bar{k} near the bouncing energy scale. The curves above only differ for very small values of \bar{k} which give negligible contributions to particle creation. Integration over \bar{k} gives the same result for all r_b not too close to the bouncing energy scale, $r_b \ll 1$.

Massive Case

In the massive minimally coupled case, the equation (4.34) reduces to

$$\phi_k'' + \left[\bar{k}^2 + r_b^2 (1 + \bar{\eta}^2) - \frac{1}{(1 + \bar{\eta}^2)^2} \right] \phi_k = 0, \quad (4.52)$$

and it can be seen that the potential term again goes to zero at infinity. The asymptotic solutions are then the same as in (4.36) and (4.37). Thus, we used (4.36) and its derivative again to place the initial conditions at $\bar{\eta}_i$ given by (4.46), being understood that this is exact only at infinity. In order to test the consistency of the choice of initial time, we evaluated the initial exact solutions along with our numerical solutions. We did this for a number of values of the parameters, with $\bar{k} < 10$ and $r_b \ll 1$, and found no inconsistency: the numerical evolution was indistinguishable from the exact solution (4.36) for sufficient early times. An example of this is shown in figure 4.4. The figure 4.3 shows the Bogoliubov coefficients in the minimal coupling case with a few different masses. It can be seen that the Bogoliubov coefficients are many orders of magnitude greater than in the conformal case, see figure 4.2. The shape of the spectrum is similar to the massless case because it is determined by the potential near the bounce, which does not depend on the mass. Another way to say this is that the mass-dependent term in the Klein–Gordon equation is only dominant away from the bounce, where the adiabatic conditions are valid, and it is therefore not effective. Note that we are not considering super-massive particles with masses near the bouncing energy scale.

Finally, as remarked before, the total particle number density for the massive and massless particles are equal, within the required precision, and they are both given in equation (4.50). In the ultra-relativistic limit,

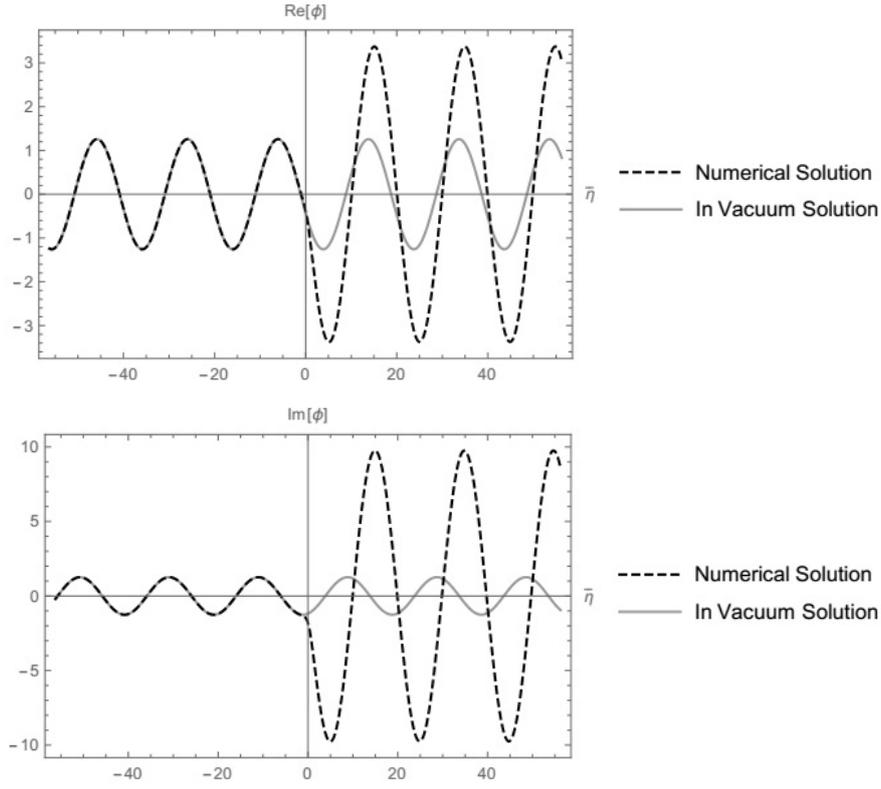


Figure 4.4: Evolution of the numerical solution (in the minimal coupling case) and the initial WKB solution (4.36) for a particular \bar{k} and r_b . Since the Klein–Gordon equation is real, the real and imaginary components of the solutions can be considered separately. It is shown that the initial conditions are consistent. Both solutions evolve together until very near the bounce where the ξ –dependent potential term becomes relevant. This is very similar to the one–dimensional potential problem in non–relativistic quantum mechanics.

the energy density is given in equation (4.51). In the non–relativistic limit, the energy density is described by a dust like fluid (equation (4.32)), namely

$$\Omega_\phi = \frac{m n}{\rho_{crit0}} = 2.1 x^3 \left(\frac{m}{m_H} \right) \left(\frac{x_b}{10^{30}} \right)^3 \times 10^6. \quad (4.53)$$

Hence, for scalars with the Higgs particle mass, any bouncing model of this type with $x_b > 10^{27}$ will produce a dust–like fluid of particles with energy density larger than the critical density today.

4.3.2 Bouncing with Radiation and Dust

In this section, we consider a model of the universe where its energy content is dominated by two fluids, dust and radiation, such that the radiation fluid dominates during the bounce and the dust fluid dominates in the far past before the bounce, and in the far future after the bounce. This is a more realistic bouncing model, not only because it takes into account the observed dark matter distribution in the universe, but also because the matter domination epoch can account for the almost scale invariant spectrum of cosmological perturbations indicated by observations.

The solution for the scale factor is given by equation (3.56). Using the interval for x_b defined at equation (3.53), we get the following interval for γ_b ,

$$3.7 \times 10^{-29} < \gamma_b \ll 7.5 \times 10^{-9}, \quad (4.54)$$

where we used the values for Ω_{m0} and Ω_{r0} discussed in section 3.3.2. In order to understand the effect of adding a dust-like fluid to the background model, let us first consider the potential term, given by (4.22) in the Klein–Gordon equation (4.21), which dictates the mode cutoff on $n_k^{(i,f)}$. This is a decreasing function of $\bar{\eta}$ with maximum at $\bar{\eta} = 0$,

$$V \Big|_{\bar{\eta}=0} = 1 + 2\gamma_b. \quad (4.55)$$

Within the allowed interval (4.54), we see that the presence of dust does not change significantly the maximum, which will be approximately the same for this whole interval. Therefore, the cutoff does not change significantly in the presence of dust.

To calculate the Bogoliubov coefficients, we follow the same algorithm as in the pure radiation case. Now, however, the mass-term in the Klein–Gordon equation has a different behavior which precludes us from using (4.36) as asymptotic vacuum solutions to place the initial conditions. Following [71], we find that the first order WKB solutions to equation (4.21) with conformal coupling and scale factor (3.56), in the case of massive particles, are

$$\phi_k^i(\bar{\eta}) = \left(2\sqrt{\bar{k}^2 + r_b^2 \gamma_b^2 \bar{\eta}^4}\right)^{-1/2} \exp \left\{ -\frac{i\bar{\eta}}{3} \sqrt{\bar{k}^2 + r_b^2 \gamma_b^2 \bar{\eta}^4} \left[1 + 2 {}_2F_1 \left(\frac{3}{4}, 1; \frac{5}{4}; -\frac{r_b^2 \gamma_b^2 \bar{\eta}^4}{\bar{k}^2} \right) \right] \right\}, \quad \bar{\eta} < 0, \quad (4.56)$$

$$\phi_k^f(\bar{\eta}) = \left(2\sqrt{\bar{k}^2 + r_b^2 \gamma_b^2 \bar{\eta}^4}\right)^{-1/2} \exp \left\{ -\frac{i\bar{\eta}}{3} \sqrt{\bar{k}^2 + r_b^2 \gamma_b^2 \bar{\eta}^4} \left[1 + 2 {}_2F_1 \left(\frac{3}{4}, 1; \frac{5}{4}; -\frac{r_b^2 \gamma_b^2 \bar{\eta}^4}{\bar{k}^2} \right) \right] \right\}, \quad \bar{\eta} > 0, \quad (4.57)$$

where ${}_2F_1$ is an Hypergeometric function [83]. In the case of massless particles, we can still use plane-wave

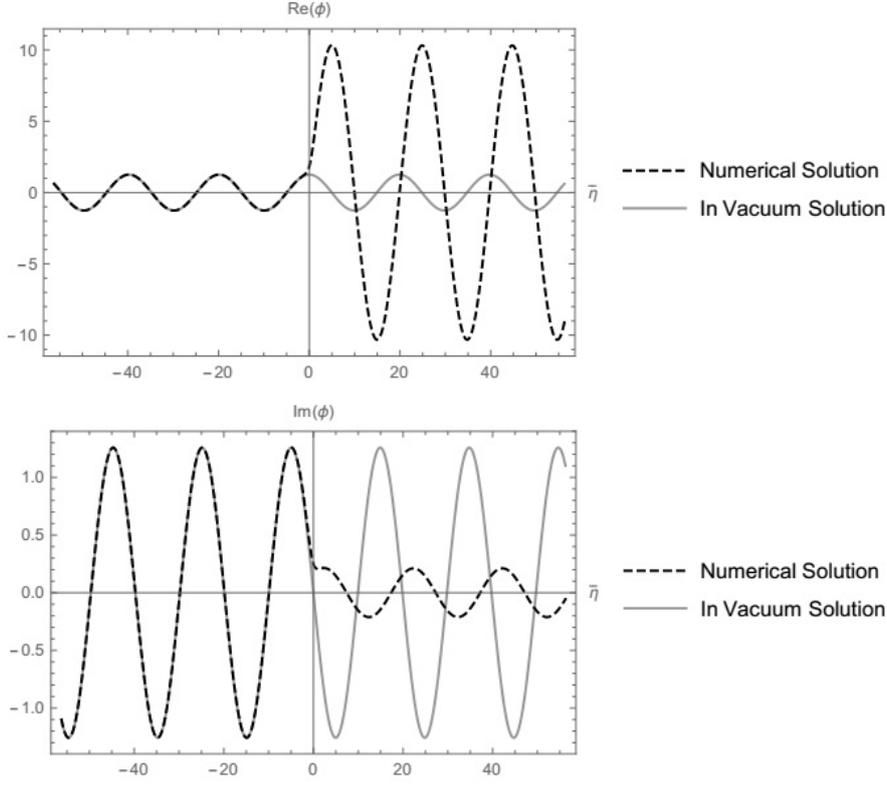


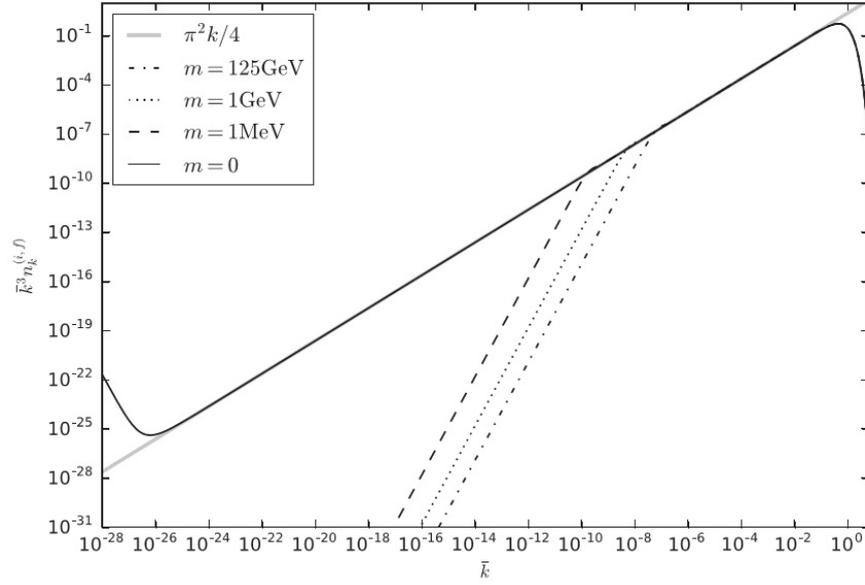
Figure 4.5: Evolution of the numerical solution (in the minimal coupling case) and the initial WKB solution (4.56) for a particular \bar{k} and r_b inside the range of integration. The same comments in figure 4.4 apply here.

solutions (4.48). A word of caution is needed here. In [4], we have found an infrared divergence in the two-fluid model for massless particles using the more reliable action-angle variables numerical approach. This happens for particles with wavelengths such that $\bar{k} < \gamma_b$. Using (4.56) and (4.56) as WKB approximations, we have found no such divergencies. The WKB approximations fail because such long-wavelength particles are more sensitive to the time-dependence of the curvature scale [71] and there is no mass term to prevent the infrared divergence (and the dust-dominated universe grows slightly faster than the radiation-dominated one, see equations (2.9) and (2.11)). This discrepancy is not present in the range of \bar{k} that we use to integrate the Bogoliubov coefficients (near the bounce energy scale, where massive and massless spectra are indistinguishable) to calculate the total particle number density. We also verified the consistency of the initial conditions inside the range of integration. An example is shown in figure 4.5. The infrared divergence is shown in figure 4.6. The infrared increase of $\beta_k^{(i,f)}$ begins at $\bar{k} < \gamma_b$, implying that the adiabatic approximation is not good in this interval.

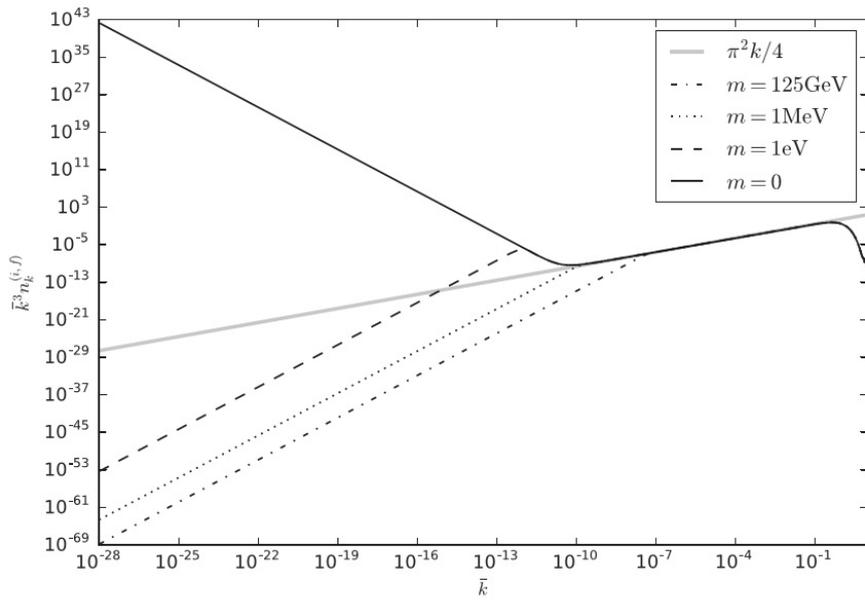
We are only interested in the minimal coupling case, since we verified that particle creation in the conformal coupling case is again very small. Apart from the infrared divergence in the massless case, we obtained the same result as in equation (4.50). Therefore, the amount of particle creation not only does not depend on the mass of the particles (except for the conformal case, of course), but also does not depend on the radiation-matter equality constant γ_b , for values within the constraint (4.54). The amount of gravitational particle creation away from

the bounce is negligible compared to that near the bounce, where the radiation fluid dominates. In particular, the fluid that dominates before radiation is not important. All that matters is the gravitational coupling and which fluid dominates during the bouncing phase. If, for instance, we bring the moment of radiation–matter equality close enough to the bounce, then the amount of particle creation becomes sensitive to γ_b . However, this happens only for values far outside the observational constraint (4.54), $\gamma_b \gg 10^{-9}$. Hence, the results of the last section for the number density of particles created and their energy densities are the same.

The infrared divergence of $n_k^{(i,f)}$ in the massless case takes place at very long wave-lengths. In figure 4.6a, for example, it starts at $\bar{k} \approx \gamma_b = 10^{-27}$, which is roughly 0.4 Mpc, but it begins with a very small amplitude $\approx 10^{-25}$. It only becomes relevant for much larger wave-lengths ≈ 108 Gpc. These modes leave the adiabatic regime at early times $\bar{k}\bar{\eta} \approx 1$, so that a contracting model with a large but finite initial time $\bar{\eta}_i$ has an infrared cutoff at $\bar{k}_i = 1/\bar{\eta}_i$. The adiabatic vacuum is therefore not well defined for long wave-lengths. These modes, however, correspond to wavelengths larger than the initial time scale of the universe, and one could simply choose to neglect these non-causal modes. If the universe is finite in volume, there is also a maximum wavelength and the infrared divergence should disappear. Alternatively, this divergence can be seen as a constraint on the initial conditions of the model. Also note that, since the equation for the Mukhanov–Sasaki variables are essentially identical to the Klein–Gordon equation [43], a similar feature is found in the semi-classical approach to cosmological perturbations generated by a quantum scalar field. The matter–bounce scenario thus naturally leads to a heavy production of long wave-length massless particles, unless constraints on initial time and/or volume are placed.



(a) $\gamma_b = 10^{-27}$



(b) $\gamma_b = 10^{-11}$

Figure 4.6: The Bogoliubov coefficients in the minimal coupling case in the model with radiation and dust. These pictures are taken from [4]. In the top figure, $\gamma_b = 10^{-27}$. In the bottom, $\gamma_b = 10^{-11}$, therefore the bounce is more shallow, which means that the bouncing phase ends closer to nucleosynthesis. Both pictures present similar spectra, however, the infrared divergence for massless particles is more evident in the latter case. Near the bouncing energy scale, massive and massless spectra are indistinguishable.

Chapter 5

Conclusions

*Habe nun, ach! Philosophie,
Juristerei und Medizin,
Und leider auch Theologie
Durchaus studiert, mit heissem Bemühn.
Da steh' ich nun, ich armer Tor,
Und bin so klug als wie zuvor.*

Johann Wolfgang von Goethe, Faust.

In this thesis, we calculated the gravitational creation of scalar particles in a set of quantum cosmological bouncing models obtained from the Bohm–de Broglie interpretation of the Wheeler–DeWitt equation restricted to minisuperspace. The first model considered is a single–fluid radiation–dominated model with scale factor given by (3.57). The second, more realistic model consists of two fluids, dust and radiation, such that the radiation fluid dominates near the bounce and the dust fluid dominates in the far past and in the far future, away from the bounce. This is described by the scale factor (3.56), of which (3.57) is a particular case.

The Bogoliubov coefficients for conformally coupled scalar particles, $\xi = 1/6$, in the single radiation fluid model has exact solutions known in the literature [71, 81, 82]. However, we have also calculated numerically the Bogoliubov coefficients in order to test our algorithm. Figure 4.2 shows that our method is consistent. Proceeding to the minimal coupling case, we found that particle creation is considerably enhanced, figure 4.3, and that the final number density is not sensitive to the particle mass. This is because realistic values of the masses of the

particles are much smaller than the bouncing energy scale given by the potential at the bounce, where particle creation takes place. Moreover, although the Bogoliubov coefficients differ at the infrared, particle creation is only effective for \bar{k} near the bouncing energy scale, where the Bogoliubov coefficients are the same. Then, we went on to consider the two–fluid model. We used the same algorithm as before but with new WKB solutions (appropriate to the scale factor (3.56)) as vacuum initial conditions. Again, the minimal coupling considerably enhances particle production in comparison with the conformal coupling case. We found the same final number density as in the single radiation model. Therefore, particle creation with minimal coupling in such models not only does not depend on the mass of the particles, but it also does not depend on the nature of the fluid that dominates away from the bounce. In particular, it does not depend on the time of matter–radiation equality for values of γ_b within the observational constraint (4.54). The energy density of massless particles is given in equation (4.51). This is in general small for the allowed range of parameters. The energy density of massive particles is given in equation (4.53). In this case, for scalars with the Higgs particle mass, any bouncing model of this type with $x_b > 10^{27}$ will produce a dust–like fluid of particles with energy density larger than the critical density today. Note that this value of x_b is inside the allowed range (3.53). Therefore (4.53) gives a nontrivial constraint. Our numerical results are further confirmed in the action-angle variable approach explained in [4] throughout the text and in the appendice.

Finally, in the massless case with two fluids, there is an infrared divergence which leads to a heavy production of long wave–length massless particles, unless constraints on their initial time and/or volume are imposed. Given that photons are also massless bosons, this may have observable consequences. This calls for more research. This infrared divergence is important only for wavelengths much larger than the size of the universe. Hence, for models with a finite age and/or volume, as long as these initial conditions are consistent with constraints from standard cosmology and its puzzles, this strong infrared production disappears. The same infrared divergence must be present in the calculation of scalar cosmological perturbations in the two–fluids background considered here.

Some important omissions in this thesis include the following.

Dirac Particles

The gravitational creation of particles in bouncing models is analogous to the mechanism of preheating where a semi–period of oscillation of the classical coherent inflaton field corresponds to the bouncing of the scale factor. The literature on preheating in inflation is rather extensive and may be exploited in a bouncing context. We did some preliminary calculations following the Hamiltonian instant diagonalization (explained, for instance, in [84, 85]) for free fermions in a radiation–dominated bouncing universe with the scale factor (3.57). Apparently, gravitational creation of fermions in such model is a few orders of magnitude smaller than the

creation of scalar particles with conformal coupling for the masses we considered in this thesis. This is not surprising, since the free massless Dirac equation in a curved space–time is conformally invariant without any coupling term and, moreover, fermions are restricted by the Pauli exclusion principle. If this is confirmed, it means that these bouncing models are stable against the gravitational creation of particles subject to the Dirac equation, which may include neutrinos and the spin 1/2 components of the gravitinos. Further calculations are required though.

Interactions

We could also exploit the same algorithm used in this thesis if we add an interaction with another field such that the interaction term in the Klein–Gordon equation falls faster than the ξ –dependent potential term. In this case, we could use the same vacuum initial conditions as before. Apparently, for these interactions to have any impact on particle creation with minimal coupling, the interaction constant would have to be unusually large so that the interaction term could be of the same order of magnitude of the potential near the bounce. A more detailed calculation is required though. A similar conclusion in a different context is found in Quintin et al [78].

Back–Reaction

In this thesis, we did not consider back–reaction from particle creation in bouncing models. The issue of back–reaction in a quantum cosmological solution is a complicated problem that deserves a work of its own. In our case this would involve an understanding of field quantization in curved space in the de Broglie–Bohm interpretation. This issue is particularly important if one takes into consideration the infrared divergence for massless particles in the two–fluid model. Moreover, we found that the energy density of the massive minimally coupled particles gravitationally created may be comparable to the density of the background. In such cases, back–reaction is also expected to be relevant for the bouncing dynamics.

Appendix A

Action Angle Variables

In this thesis, we chose to present our numerical results using WKB approximations as initial conditions. Our results are further confirmed by the action–angle variables approach. For convenience, we have reproduced here the appendix in [4], where more details can be found throughout the text.

The equation of motion (4.21) describes the evolution of the modes. Its solutions oscillate when the positive terms (\bar{k}^2 or the mass term) dominate over the potential V . During this period of the evolution, the highly oscillatory behavior forbid a precise numerical calculation [86].

The usual approach to this problem is to use a WKB approximation up to a point with less oscillations, and then change for a numerical evaluation of the solutions. Although it is also possible to work with the WKB approximation passing from the oscillatory to the non–oscillatory regimes, this approach is cumbersome and can lead to wrong conclusions if care is not taken [87]. Finally, the WKB approximation describes the solution in terms of the positive and negative solutions separately. However, we are interested in the growth of the negative frequency solutions whenever we start with only positive ones.

For the reasons above we use the Action Angle (AA) variables approach, originally used in [88, 89] in this context. Here we argue that this methodology provides both an approximation method and a better suited system of equations to solve numerically. It is also particularly convenient for the computation of particle creation, since it describes both the positive and the negative frequencies solution within the same approximation scheme.

The AA variables are related to the modes through the expressions

$$q_k = \sqrt{\frac{2I}{\nu}} \sin \theta, \quad q'_k = \sqrt{2I\nu} \cos \theta \quad (\text{A.1})$$

where q_k are real solutions of (4.21). Using these variables, the equations of motion are recast as

$$\theta' = \nu - \frac{V}{\nu} \sin^2 \theta + \frac{\nu'}{2\nu} \sin 2\theta, \quad (\text{A.2})$$

$$(\ln I)' = -\frac{\nu'}{\nu} \cos 2\theta + \frac{V}{\nu} \sin 2\theta. \quad (\text{A.3})$$

Note that this choice of variables decouples the equations, that is, the evolution of the angle variable θ is independent from the adiabatic invariant I . Thus, the integral solution for I is simply,

$$I = I_0 \exp \left[- \int_{\eta_0}^{\eta} d\eta_1 \left(\frac{\nu'_1}{\nu_1} \cos 2\theta_1 - \frac{V_1}{\nu_1} \sin 2\theta_1 \right) \right]. \quad (\text{A.4})$$

To build a complex solution, we introduce another set of AA variables J and ψ , satisfying the same set above, that is,

$$\psi' = \nu - \frac{V}{\nu} \sin^2 \psi + \frac{\nu'}{2\nu} \sin 2\psi, \quad (\text{A.5})$$

$$(\ln J)' = -\frac{\nu'}{\nu} \cos 2\psi + \frac{V}{\nu} \sin 2\psi. \quad (\text{A.6})$$

from which we introduce another real field variable

$$v_k = \sqrt{\frac{2I}{\nu}} \sin \psi, \quad v'_k = \sqrt{2I\nu} \cos \psi.$$

Thus, the complex solution can be written as

$$\phi_k = \frac{q_k + iv_k}{2i} = \frac{1}{i\sqrt{2\nu}} \left(\sqrt{I} \sin \theta + i\sqrt{J} \sin \psi \right) \quad (\text{A.7})$$

$$\phi'_k = \frac{q'_k + iv'_k}{2i} = \frac{1}{i} \sqrt{\frac{\nu}{2}} \left(\sqrt{I} \cos \theta + i\sqrt{J} \cos \psi \right) \quad (\text{A.8})$$

The mode normalization conditions

$$i (\phi_k^* \phi'_k - \phi_k^{*'} \phi_k) = 1,$$

imply

$$\sqrt{I J} \sin (\psi - \theta) = 1. \quad (\text{A.9})$$

Note that the normalization condition is proportional to the Wronskian of the real and imaginary solutions, that is,

$$\mathcal{W}(q_k, v_k) = 2\sqrt{I J} \sin (\psi - \theta) = 2.$$

Considering the adiabatic limit ($V \rightarrow 0$ and $\nu'/\nu \rightarrow 0$), the solutions are simply

$$\begin{aligned} I &= I_0, & J &= J_0 \\ \theta &= \theta_0 + \int d\eta \nu, & \psi &= \psi_0 + \int d\eta \nu. \end{aligned} \quad (\text{A.10})$$

In this limit, the choices $\psi_0 = \theta_0 + \pi/2$ and $I_0 = J_0 = 1$ satisfy the normalization condition in (A.9), and we obtain the correct adiabatic vacuum, namely

$$\phi_k = \frac{1}{\sqrt{2\nu}} \exp\left(-i \int d\eta \nu\right). \quad (\text{A.11})$$

It is worth emphasizing that in the ultraviolet limit ($k \rightarrow \infty$), the same approximate solution above applies.

The potential V goes to zero in the limits $\eta \rightarrow \pm\infty$, therefore, we can choose two initial conditions, each one matching the adiabatic vacuum in the limit. Looking at the integral solution in (A.4), it is easy to see that the solutions

$$I^{(i)} = \exp\left[-\int_{-\infty}^{\eta} d\eta_1 \left(\frac{\nu'_1}{\nu_1} \cos 2\theta_1^{(i)} - \frac{V_1}{\nu_1} \sin 2\theta_1^{(i)}\right)\right] \quad (\text{A.12})$$

$$J^{(i)} = \exp\left[-\int_{-\infty}^{\eta} d\eta_1 \left(\frac{\nu'_1}{\nu_1} \cos 2\psi_1^{(i)} - \frac{V_1}{\nu_1} \sin 2\psi_1^{(i)}\right)\right] \quad (\text{A.13})$$

and the condition

$$\lim_{\eta \rightarrow -\infty} \psi^{(i)} - \theta^{(i)} = \pi/2$$

produce the right solution matching the asymptotic in the $\eta \rightarrow -\infty$ limit, namely, $\phi_k^{(i)}$. Analogously, for the $\eta \rightarrow +\infty$ limit we obtain the solution $\phi_k^{(f)}$ through the following AA variables

$$I^{(f)} = \exp\left[\int_{\eta}^{\infty} d\eta_1 \left(\frac{\nu'_1}{\nu_1} \cos 2\theta_1^{(f)} - \frac{V_1}{\nu_1} \sin 2\theta_1^{(f)}\right)\right], \quad (\text{A.14})$$

$$J^{(f)} = \exp\left[\int_{\eta}^{\infty} d\eta_1 \left(\frac{\nu'_1}{\nu_1} \cos 2\psi_1^{(f)} - \frac{V_1}{\nu_1} \sin 2\psi_1^{(f)}\right)\right], \quad (\text{A.15})$$

and the condition

$$\lim_{\eta \rightarrow \infty} \psi^{(f)} - \theta^{(f)} = \pi/2.$$

Both solutions $\phi_k^{(i)}$ and $\phi_k^{(f)}$ provide a well defined adiabatic vacuum for $\eta \gg 1$ accordingly. In these intervals $V/\nu^2 \ll 1$ and $\nu'/\nu \ll 1$ and consequently

$$I \approx 1, \quad J \approx 1, \quad \psi - \theta \approx \frac{\pi}{2}$$

Particularly, this means that both solutions remain close to the form given in (A.11) during this time interval.

Finally, we need to compute the products between these two solutions. The Bogoliubov coefficients are given by,

$$\alpha_k^{(i,f)} = i \left(\phi_k^{(i)*} \phi_k^{(f)'} - \phi_k^{(i)'} \phi_k^{(f)*} \right), \quad (\text{A.16})$$

$$\beta_k^{(i,f)} = i \left(\phi_k^{(i)} \phi_k^{(f)'} - \phi_k^{(i)'} \phi_k^{(f)} \right). \quad (\text{A.17})$$

Writing these expression in terms of the real solutions we get,

$$\alpha_k^{(i,f)} = -\frac{1}{2} \left[\mathcal{W}(q_k^{(i)}, v_k^{(f)}) + \mathcal{W}(q_k^{(f)}, v_k^{(i)}) \right] + \frac{i}{2} \left[\mathcal{W}(q_k^{(i)}, q_k^{(f)}) + \mathcal{W}(v_k^{(f)}, v_k^{(i)}) \right] \quad (\text{A.18})$$

and

$$\beta_k^{(i,f)} = +\frac{1}{2} \left[\mathcal{W}(q_k^{(i)}, v_k^{(f)}) - \mathcal{W}(q_k^{(f)}, v_k^{(i)}) \right] - \frac{i}{2} \left[\mathcal{W}(q_k^{(i)}, q_k^{(f)}) - \mathcal{W}(v_k^{(f)}, v_k^{(i)}) \right] \quad (\text{A.19})$$

Since these Wronskians are constant we can evaluate them at any time. In the limit $\eta_f \gg 1$ we obtain,

$$\left| \alpha_k^{(i,f)} \right|^2 = \frac{1}{4} \left(I^{(i)} + J^{(i)} + 2 \right) \Big|_{\eta=\eta_f}, \quad (\text{A.20})$$

$$\left| \beta_k^{(i,f)} \right|^2 = \frac{1}{4} \left(I^{(i)} + J^{(i)} - 2 \right) \Big|_{\eta=\eta_f}. \quad (\text{A.21})$$

The result above shows the convenience of this approach. The adiabatic invariants $I^{(i)}$ and $J^{(i)}$ provide the value of $\beta_k^{(i,f)}$ when evaluated at η_f . It is also worth noting that although $I^{(i)}$ and $J^{(i)}$ are adiabatic invariants, their logarithm is not. In the initial regime $\eta \ll 1$, $I^{(i)}$ can be approximated as

$$I^{(i)} \approx 1 - \int_{-\infty}^{\eta} d\eta_1 \left(\frac{\nu_1'}{\nu_1} \cos 2\theta_1^{(i)} - \frac{V_1}{\nu_1} \sin 2\theta_1^{(i)} \right), \quad (\text{A.22})$$

showing that, as long as $V/\nu \ll 1$ and $\nu'/\nu \ll 1$, $I^{(i)} \approx 1$ provides a good approximation for this variable, where the same reasoning applies to $J^{(i)}$.

During the oscillatory regime, we can also obtain the first order approximation of the integrals $I^{(i)}$ and $J^{(i)}$ as [90]

$$\ln \left(I^{(i)} \right) \approx -\frac{\nu'}{2\nu^2} \sin 2\theta^{(i)} - \frac{V}{2\nu^2} \cos 2\theta^{(i)}, \quad (\text{A.23})$$

$$\ln \left(J^{(i)} \right) \approx -\frac{\nu'}{2\nu^2} \sin 2\psi^{(i)} - \frac{V}{2\nu^2} \cos 2\psi^{(i)}. \quad (\text{A.24})$$

Similarly, for $\theta^{(i)}$ and $\psi^{(i)}$ we get

$$\theta^{(i)} \approx \sigma - \frac{\nu'}{4\nu^2} \cos 2\theta^{(i)} + \frac{V}{4\nu^2} \sin 2\theta^{(i)}, \quad (\text{A.25})$$

$$\psi^{(i)} \approx \frac{\pi}{2} + \sigma - \frac{\nu'}{4\nu^2} \cos 2\psi^{(i)} + \frac{V}{4\nu^2} \sin 2\psi^{(i)}, \quad (\text{A.26})$$

where

$$\sigma = \int d\eta \nu \left(1 - \frac{V}{\nu^2} \right). \quad (\text{A.27})$$

In the numerical calculations, we used the approximations above. We set the initial time for each mode at the point $\eta < -1$ where

$$\text{MAX}(|V/\nu^2|, |\nu'/\nu^2|) = \epsilon, \quad (\text{A.28})$$

where ϵ controls the precision required.

During the non-adiabatic evolution, we can compute the solutions for (A.2) and (A.3) in two cases. Ignoring all terms but the ν'/ν we get

$$\theta = \cot^{-1} \left(\cot \theta_0 \frac{\nu_0}{\nu} \right), \quad (\text{A.29})$$

$$I = I_0 \left(\sin^2 \theta_0 \frac{\nu}{\nu_0} + \cos^2 \theta_0 \frac{\nu_0}{\nu} \right). \quad (\text{A.30})$$

When evolving through the bounce phase, since ν is an even function and considering $\eta_0 < 0$, we obtain $I(-\eta_0) = I(\eta_0)$, where subindex $_0$ denotes some arbitrary initial time. In short, for an even ν , the evolution through the bounce for modes for which ν'/ν^2 dominates, makes I return to the same value it started.

The second case, where the term V/ν is the only relevant one, have the following solutions

$$\theta = \cot^{-1} \left[\cot \theta_0 + f(\eta, \eta_0) \right], \quad (\text{A.31})$$

$$I = I_0 \left[1 + f(\eta, \eta_0) \left(f(\eta, \eta_0) \sin^2 \theta_0 + \sin 2\theta_0 \right) \right], \quad (\text{A.32})$$

where

$$f(\eta, \eta_0) = \int_{\eta_0}^{\eta} d\eta_1 \frac{V_1}{\nu_1}.$$

The solution above is valid for both I and J . Remembering that θ and ψ have a $\pi/2$ difference, if $\theta_0 = 0$, then $I = I_0$ and $J = J_0 (1 + f(\eta, \eta_0)^2)$. Therefore, the adiabatic invariants have their amplitude increased by a factor of $1 + f(\eta, \eta_0)^2$.

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