Parametrization, Quantization, and Observables

Bachelor science project report

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Abstract

In this article I follow the method of parametrization, discuss the choice of time, define constraints, construct Hamiltonians, and quantize classical equations to achieve a quantum model of different systems. I indicate that an action principle must be parametrization invariant, and also parametrize dynamical systems equations. Then, I try to construct Dirac observables and also find their quantum mechanical form. In the end, I discover the Friedmann universe and solve the equations that are necessary in order to define this particular model of our universe. One can see from the title of this article that three subjects constitute the body of our discussions:

Parametrization: The first concept of interest is parametrization. It is crucial to know what will happen if we apply parametrization to a system. Parametrization invariance gives us the key to open the door that leads to the unknown dungeons of *quantum gravity*. Thanks to parametrization invariance, the equations of our theory will become background-independent, and also the laws of physics will maintain their form under coordinate transformations.

Quantization: The second significant concept in this article is the act of quantization. This is a procedure in which we describe a physical Hilbert space, turn specific quantities into operators, and then write down the equations describing the system. We quantize our theories to become able to explain our theories in the territory of quantum mechanics. Many people believe that if we think in terms of quantum mechanics, then the answers to our questions will become more and more accessible.

Observables: The final concept is the observables. There is a simple and clear definition of an observable in physics: An observable is a physical quantity that can be measured. We are interested in these kinds of quantities because the process of measurement is important to understand, especially in quantum mechanics. To obtain observables, we use the constraints, gauge conditions, and the Hamiltonian of our system of interest.

All of the above concepts are used and discussed through this article.

Keywords : Parametrization, Action, Constraint, Invariance, Hamiltonian, Observable, Quantization.

Contents

1 Introduction

It was at the year 1915 when Albert Einstein first discovered a way to define gravity not as a force, but simply as the product of bent four-dimensional spacetime. He called this newly formed knowledge about our nature, *general relativity*. The theory of GR (general relativity) is what one calls a classical theory. All other interactions are now described in the quantum framework. So if all other interactions can be explained by quantum mechanics, why gravitation is the exceptional case so far? If one is interested to become able to write down a unification of all interactions in nature, then gravity should be quantized. The sections which are covered in this article can be used to understand 'quantum gravity'. What is quantum gravity? This theory is one of the most remarkable ideas that a lot of people are working on as we speak. The goal of this theory is to become able to describe GR in a quantum manner, and therefore make gravity compatible with the quantum mechanical realm. When we say quantum gravity, we mean a theory in which the superposition principle is applied to the gravitational field.

In each section of this article, we consider two different approaches to the problem which we are dealing with: The classical approach, and the quantum theory. In section 2, our goal is to understand the method of parametrization and to observe how different quantities behave during this process. Also, deriving Hamiltonian constraints is another problem which we consider in this section. In the third part, we are going to discuss the act of construction of Dirac observables. What are Dirac observables? We sure are going to try to answer that question. The final part is somehow a great example that indicates how the things we already learned through sections 2 and 3, are going to come in handy to solve some important equations about our universe. When working on Friedmann universe, we can see that the behavior of some of the parameters of our universe can be understood easier than one may have thought. However, we are going to detect some serious problems which place a wall in front of our borders of knowledge.

All of the sections in this article are going to be discussed in a way that the reader could be able to grasp a general understanding of each one of these sections. Therefore, we will try to express the concept and the mathematics needed for our purpose.

2 Parametrized and relational systems

The key aspect in this section is the *reparametrization invariance*. Such invariance properties are often referred to as 'general covariance'. General covariance consists of the invariance of the form of physical laws under arbitrary differentiable coordinate transformations. It actually implies a formalism in which laws of physics maintain the same form under a specified set of transformation. General covariance should be interpreted as the absence of absolute structure, which is also called 'background independence'. This section follows chapter 3 of [1] in concepts and formulation.

2.1 Parametrized non-relativistic particle

We consider a point particle that is free and no potential is applied on its path of movement. The action for a point particle is simply

$$S[q(t)] = \int_{t_1}^{t_2} \mathrm{d}t\ L\left(q, \frac{\mathrm{d}q}{\mathrm{d}t}\right). \tag{1}$$

We introduce a formal time parameter τ (label time). The Newton's absolute time t (the elevate) is then a dynamical variable same as q. Using $\mathrm{d}t = \frac{\mathrm{d}t}{\mathrm{d}\tau}\mathrm{d}\tau$ leaves us with the action

$$S[q(\tau), t(\tau)] = \int_{\tau_1}^{\tau_2} \mathrm{d}\tau\ \dot{t}L\left(q, \frac{\dot{q}}{\dot{t}}\right) =: \int_{\tau_1}^{\tau_2} \mathrm{d}\tau\ \tilde{L}\left(q, \dot{q}, \dot{t}\right). \tag{2}$$

Note that dot denotes to derivative with respect to τ. The Lagrangian $\tilde{L}$ that appeared here, is called the *homogeneous Lagrangian*, which is homogeneous in the velocities ($\dot{t}$ and $\dot{q}$ are velocities here). The homogeneous Lagrangian has a behavior that is

$$\tilde{L}\left(q, \lambda\dot{q}, \lambda\dot{t}\right) = \lambda\tilde{L}\left(q, \dot{q}, \dot{t}\right), \tag{3}$$

where λ is an arbitrary parameter.

Now we are willing to consider a time reparametrization. This reparametrization is indicated by $\tau \to \tilde{\tau} = f(\tau)$. One can rewrite the action in which τ is reparametrized. It is

$$S = \int_{\tau_1}^{\tau_2} \mathrm{d}\tau\ L\left(q, \dot{q}\right) = \int_{\tilde{\tau_1}}^{\tilde{\tau_2}} \frac{\mathrm{d}\tilde{\tau}}{\dot{f}} L\left(q, \frac{\mathrm{d}q}{\mathrm{d}\tilde{\tau}}\dot{f}\right) = \int_{\tilde{\tau_1}}^{\tilde{\tau_2}} \mathrm{d}\tilde{\tau}\ L\left(q, \frac{dq}{d\tau}\right). \tag{4}$$

As we can see, the action remained invariant under time reparametrization (obviously the form of action did not change), and therefore the equations of motion will not change their form. It is important to know whether any quantity remains invariant under reparametrization or not.

The canonical momentums can be constructed by differentiating the homogeneous Lagrangian. They are given by (take a look at (2) to remember the connection between the regular Lagrangian and the homogeneous Lagrangian)

$$\tilde{p_q} = \frac{\partial\tilde{L}}{\partial\dot{q}} = \dot{t}\frac{\partial L}{\partial(\dot{q}/\dot{t})}\frac{1}{\dot{t}} = p_q, \tag{5}$$

$$
\begin{aligned}
p_t = \frac{\partial \tilde{L}}{\partial \dot{t}} = \frac{\partial(\dot{t}L)}{\partial \dot{t}} &= L\left(q, \frac{\dot{q}}{\dot{t}}\right) + \dot{t}\frac{\partial L(q, \dot{q}/\dot{t})}{\partial \dot{t}} \\
&= L\left(q, \frac{\dot{q}}{\dot{t}}\right) - \frac{\dot{q}}{\dot{t}^2}\dot{t}\frac{\partial L(q, \dot{q}/\dot{t})}{\partial(\dot{q}/\dot{t})} \\
&= L\left(q, \frac{\mathrm{d}q}{\mathrm{d}t}\right) - \frac{\mathrm{d}q}{\mathrm{d}t}\frac{\partial L(q, \mathrm{d}q/\mathrm{d}t)}{\partial(\mathrm{d}q/\mathrm{d}t)} = -H.
\end{aligned} \tag{6}
$$

The Hamiltonian corresponding to $\tilde{L}$ is found to be

$$
\tilde{H} = \tilde{p_q}\dot{q} + p_t\dot{t} - \tilde{L} = \dot{t}(H + p_t). \tag{7}
$$

From equation (6) one can see that p_t is equal to $-H$. Then we can define a new kind of Hamiltonian which can be written as

$$
\begin{aligned}
H_S &= H + p_t, \\
H_S &\approx 0.
\end{aligned} \tag{8}
$$

The above equation shows that the H_s vanishes as a constraint (H_s is called *the super-Hamiltonian*). It means under the constraint $H = -p_t$, The super Hamiltonian value is zero. What is the use of H_s? We can use the super Hamiltonian to write the new action principle as

$$
S = \int_{\tau_1}^{\tau_2} \mathrm{d}\tau(p_q\dot{q} + p_t\dot{t} - \dot{t}H_S), \tag{9}
$$

$$
\dot{t} = \frac{\partial(NH_S)}{\partial p_t} = N, \tag{10}
$$

where N is a Lagrangian multiplier which is called the *Lapse function*. The lapse function gives the rate of change of Newton's time with respect to the label time. So the action will become

$$
S = \int_{\tau_1}^{\tau_2} \mathrm{d}\tau(p_q\dot{q} + p_t\dot{t} - NH_S). \tag{11}
$$

If we were to quantize a constraint like (8), we would write the super Hamiltonian as an operator. Then the constraint equation would be translated into

$$
\hat{H}_S\psi = 0, \tag{12}
$$

where $\hat{H_S}$ denotes the super-Hamiltonian operator and ψ is the wave function. The quantum version of (8) becomes

$$
\left(\hat{H} - i\hbar\frac{\partial}{\partial t}\right)\psi(q,t) = 0, \tag{13}
$$

in which we have just rewritten the super Hamiltonian in terms of the regular Hamiltonian and the momentum operator $\hat{p}_t$. As we know equation (13) is just the Schrodinger equation.

2.2 Parametrized field theories

Consider a scalar field in Minkowski space $\phi(X^\mu)$, where the standard inertial coordinates are $X^\mu \equiv (T, X^a)$. As we know, X^μ is a contravariant vector. We now introduce arbitrary coordinates $x^\mu \equiv (t, x^a)$ and let X^μ depend parametrically on x^μ. The functions $X^\mu(x^\nu)$ describe a family of hypersurfaces in Minkowski space parametrized by $x^0 \equiv t$. The standard actoin for a scalar field may be written as

$$S = \int \mathrm{d}^4X \; L\left(\phi, \frac{\partial \phi}{\partial X^\mu}\right) = \int \mathrm{d}^4x \; \tilde{L}, \tag{14}$$

where

$$\tilde{L}\left(\phi, \phi_{,a}, \dot{\phi}; X^\mu_{,a}, \dot{X}^\mu\right) = JL\left(\phi, \phi_{,\nu}, \frac{\partial x^\nu}{\partial X^\mu}\right), \tag{15}$$

in which J denotes the Jacobi determinant of the X with respect to the x, and $\phi_{,\nu} \equiv \frac{\partial \phi}{\partial x^\nu}$.

Consider the Hamiltonain density $\tilde{H}$ corresponding to $\tilde{L}$ with respect to ϕ, which is

$$\tilde{H} = \tilde{p_\phi}\dot{\phi} - \tilde{L} = J\frac{\partial L}{\partial \dot{\phi}}\dot{\phi} - JL \tag{16}$$

$$= J\frac{\partial x^0}{\partial X^\mu}\left(\frac{\partial L}{\partial(\partial\phi/\partial X^\mu)}\frac{\partial \phi}{\partial X^\nu} - \delta^\mu_\nu L\right)\dot{X}^\nu \tag{17}$$

$$\equiv J\frac{\partial x^0}{\partial X^\mu}T^\mu{}_\nu \dot{X}^\nu, \tag{18}$$

where as we can see a new tensor seems to appear here. The $T^\mu{}_\nu$ tensor is called the *energy-momentum tensor*, which describes the density of energy and momentum in spacetime. Note that the energy-momentum tensor can be derived from the Lagrangian. The Jacobi determinant is written as

$$J = \epsilon_{\rho\nu\lambda\sigma}\frac{\partial X^\rho}{\partial x^0}\frac{\partial X^\nu}{\partial x^1}\frac{\partial X^\lambda}{\partial x^2}\frac{\partial X^\sigma}{\partial x^3}. \tag{19}$$

Both Jacobi determinant and energy-momentum tensor do not depend on the 'kinematical velocities' $\dot{X}^\mu$. It implies that if one is interested in constructing these two quantities, it can be done by using only the geometrical coordinates and the scalar field. The energy-momentum tensor is put into work if one wants to write the Einstein field equations in the GR (general relativity) framework.

According to (18), as a generalized form of (7), one may write the kinematical momenta Π_ν via the constraint

$$H_\nu := \Pi_\nu + J\frac{\partial x^0}{\partial X^\mu}T^\mu{}_\nu \approx 0. \tag{20}$$

By knowing the relation between the Hamiltonian and the Lagrangian, one can rewrite the action (14) in the form of

$$S = \int \mathrm{d}^4x \; (\tilde{p}_\phi\dot{\phi} - \tilde{H}). \tag{21}$$

Inserting (18) for $\tilde{H}$ and constraints (20) with Lagrangian multipliers N^ν, gives us the action as

$$S = \int \mathrm{d}^4x\ (\tilde{p}_\phi \dot{\phi} + \Pi_\nu \dot{X}^\nu - N^\nu H_\nu). \tag{22}$$

As we can see, it is analogous to (11).

We could decompose (20) into orthogonal and parallel vectors to the hypersurfaces $x^0 = \mathit{constant}$. The normal vector is n^μ (where $\eta_{\mu\nu} n^\mu n^\nu = -1$), and the tangential vector is introduced as $X^\nu_{,a} \equiv \frac{\partial X^\nu}{\partial x^a}$ (which obeys $n_\nu X^\nu_{,a} = 0$). So the orthogonal and tangential constraints will be

$$H_\perp := H_\nu n^\nu \approx 0, \tag{23}$$

$$H_a := H_\nu X^\nu_{,a} \approx 0. \tag{24}$$

Equations (23) and (24) are called Hamiltonian constraint and momentum constraints, respectively. The momentum constraints are also called diffeomorphism constraints, because they can generate infinitesimal diffeomorphisms. One might ask: What is a diffeomorphism? A diffeomorphism is typically presented as a smooth, differentiable, invertible map between manifolds. After applying (23) and (24), the action (22) becomes

$$S = \int \mathrm{d}^4x\ (\tilde{p_\phi} \dot{\phi} + \Pi_\nu \dot{X}^\nu - N H_\perp - N^a H_a). \tag{25}$$

We mentioned Lagrangian multipliers earlier. To use the method of Lagrangian multipliers for finding the value of $\dot{X}^\nu$, we should determine the Lagrangian multipliers by varying the action with respect to Π_ν, and set this variation equal to zero. We substitute H_ν from equation (20) in Equations (23) and (24). Then taking the variation of constraints with respect to Π_ν gives us the result as

$$\left(\frac{\partial}{\partial \Pi_\nu}\right) H_\perp = n^\nu, \quad \left(\frac{\partial}{\partial \Pi_\nu}\right) H_a = X^\nu_{,a} \tag{26}$$

then from the procedure we described above, we obtain

$$\dot{X}^\nu =: t^\nu = N n^\nu + N^a X^\nu_{,a}. \tag{27}$$

To have a geometrical understanding of the things mentioned above, think of $\dot{X}^\nu$ as a vector that points from a point with spatial coordinates x^a on $t =$ constant to a point with the same coordinates on a neighbouring hypersurface $t + dt =$ constant. N is called the *lapse function*, and Ndt determines the pure temporal distance between the hypersurfaces. Also, N^a is a vector that points from a point with coordinates x^a on $t =$ constant to the point on the same hypersurface from which the normal is erected to reach the point with the same coordinates x^a on $t + dt =$ constant. It is called the *shift vector*.

So far, we were working on Minkowski space. One can also choose an arbitrary curved background space-time with the metric $g_{\mu\nu}$. The spatial metric induced on the hypersurfaces is denoted by h_{ab}, that is

$$h_{ab} = g_{\mu\nu} \frac{\partial X^\mu}{\partial x^a} \frac{\partial X^\nu}{\partial x^b}. \tag{28}$$

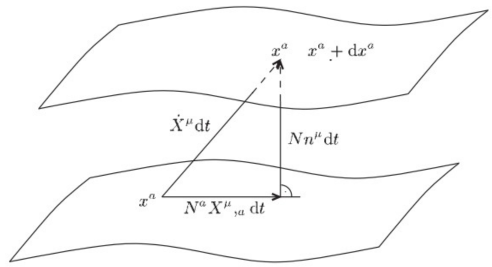

Figure 1: Geometric interpretation of lapse and shift between hypersufaces t and $t + dt$. (Kiefer, C. (2012). Quantum Gravity. Oxford.)

The four-dimensional line element can be written as

$$\begin{aligned} \mathrm{d}s^2 &= g_{\mu\nu}\mathrm{d}x^\mu \mathrm{d}x^\nu = -N^2\mathrm{d}t^2 + h_{ab}(\mathrm{d}x^a + N^a\mathrm{d}t)(\mathrm{d}x^b + N^b\mathrm{d}t) \\ &= (h_{ab}N^aN^b - N^2)\mathrm{d}t^2 + 2h_{ab}N^a\mathrm{d}x^b\mathrm{d}t + h_{ab}\mathrm{d}x^a\mathrm{d}x^b. \end{aligned} \tag{29}$$

The action (25) is invariant under reparametrizations below (parametrization of time and spatial coordinate)

$$\begin{aligned} &x^0 \to x^{0'} = x^0 + f(x^a), \\ &x^a \to x^{a'} = g(x^b), \end{aligned} \tag{30}$$

where f and g are arbitrary differentiable functions.

An example of the procedure above, is the case of a massless scalar field on (1+1)-dimensional Minkowski spacetime. Its Lagrangian is

$$L\left(\phi, \frac{\partial\phi}{\partial T}, \frac{\partial\phi}{\partial X}\right) = -\frac{1}{2}\eta^{\mu\nu}\frac{\partial\phi}{\partial X^\mu}\frac{\partial\phi}{\partial X^\nu} = \frac{1}{2}\left[\left(\frac{\partial\phi}{\partial T}\right)^2 - \left(\frac{\partial\phi}{\partial X}\right)^2\right], \tag{31}$$

where $\eta^{\mu\nu} = \mathrm{diag}\ \{\text{-1,1,1,1}\}$ (It is the ordinary metric of the Minkowski space). According to (19), for the Jacobi determinant we have (here there are only two standard inertial coordinates and two arbitrary coordinates instead of four, which are T and X)

$$J = \dot{T}X' - T'\dot{X}, \tag{32}$$

where prime denotes differentiation with respect to x. The relation $\eta_{\mu\nu}n^\mu n^\nu = -1$, gives us the condition on the normal vector (n) components, which is

$$-(n^T)^2 + (n^X)^2 = -1. \tag{33}$$

These components are given by the following relations (which of course respect the condition above)

$$n^T = \frac{X'}{\sqrt{X'^2 - T'^2}}, \quad n^X = \frac{T'}{\sqrt{X'^2 - T'^2}}. \tag{34}$$

At this point, we should ask ourselves what is the good thing about knowing the normal vectors? What is there to achieve? Well, if we remember the Hamiltonian constraints (23) and (24), it is clear that we can write down these two constraints using the relations we have already written down. One can find these constraints to be

$$H_\perp = \frac{1}{\sqrt{X'^2 - T'^2}}\Big(X'\Pi_T + T'\Pi_X + \frac{1}{2}(\tilde{p}_\phi^2 + \phi'^2)\Big), \tag{35}$$

$$H_1 = T'\Pi_T + X'\Pi_X + \phi'\tilde{p_\phi}. \tag{36}$$

It is obvious that in this case, Π_X and Π_T enter the Hamiltonian constraint *linearly*. So this is a theory which is intrinsically reparametrization invariant, that is, a theory which is background independent. Background independence is a condition that requires the defining equations of a theory to be independent of the actual shape of spacetime and the value of various fields within it.

Now let's begin the quantization of the parametrized field theory we discussed earlier. Our approach here is somehow just a brief procedure to give the reader a glance at what does the quantization may look like. We shall begin the quantization by introducing the formal commutators

$$[X^\mu(x), \Pi_\nu(y)] = i\hbar\delta^\mu_\nu\delta(x-y), \tag{37}$$

and

$$[\phi(x), \tilde{p}_\phi(y)] = i\hbar\delta(x-y). \tag{38}$$

Again from (23) and (24), one can get the quantum constraints according to Dirac's prescription

$$H_\perp\Psi[\phi(x), X^\mu(x)] = 0, \tag{39}$$

$$H_1\Psi[\phi(x), X^\mu(x)] = 0. \tag{40}$$

In general, the canonical momentum operator in quantum mechanics is indicated by

$$\hat{\Pi}_{X^a} = -i\hbar\frac{\delta}{\delta X^a}. \tag{41}$$

In the above example of free scalar field, one can construct the constraints which are operating on the wave funciton. Applying these constraints on wave functions give us the equations

$$\begin{aligned} H_\perp\Psi = \frac{1}{\sqrt{X'^2 - T'^2}}\Big(& -i\hbar X'(x)\frac{\delta}{\delta T(x)} - i\hbar T'(x)\frac{\delta}{\delta X(x)} \\ &+ \frac{1}{2}\Big[-\hbar^2\frac{\delta^2}{\delta\phi(x)\delta\phi(x)} + \phi'^2(x)\Big]\Big)\Psi[\phi(x), T(x), X(x)] = 0, \end{aligned} \tag{42}$$

$$H_1\Psi = \frac{\hbar}{i}\Big(T'(x)\frac{\delta}{\delta T(x)} + X'\frac{\delta}{\delta X(x)} + \phi'(x)\frac{\delta}{\delta\phi(x)}\Big)\Psi = 0. \tag{43}$$

The above equations are different from the equations that one would get from the standard Lagrangian (31) or its corresponding action. The reason is that the wave functional usually evolves along the flat hypersurfaces T = constant only, whereas in the parametrized version it can be evolved along any family of space-like hypersurfaces. The latter description is also called a 'many-fingered time' or 'bubble-time' description.

So far, we discussed parametrization. Consider the Schrodinger equation for the massless scalar field

$$i\hbar \frac{\partial \Psi}{\partial T} = H\Psi. \tag{44}$$

We choose $x = X$ as a coordinate on the hypersurfaces and evolve the wave functionals along hypersurfaces that are described by $T(x) = T_0 \in (-\infty, \infty)$. There can be several equations derived from (42) and (43). By applying equation (42), we can write the Schrodinger equation as

$$i\hbar \frac{\partial \Psi}{\partial T_0} = \frac{1}{2} \int \mathrm{d}X \bigg(-\hbar^2 \frac{\delta^2}{\delta \phi^2(x)} + \left[\frac{\partial \phi}{\partial X} \right]^2 \bigg) \Psi. \tag{45}$$

The interpretation of momentum constraint can be recognized from (43). One can perform an infinitesimal coordinate transformation on T = constant as the form of $x \longrightarrow \bar{x} = x + \delta N^1(x)$, to get

$$T(x) \longrightarrow T\left(x + \delta N^1(x)\right) = T(x) + T'(x)\delta N^1(x), \tag{46}$$

and similar equations for $X(x)$ and $\phi(x)$. Now for the wave functional, the transformation we considered yields

$$\begin{aligned} \Psi \longrightarrow & \Psi[T(x) + T'(x)\delta N^1(x), ...] = \Psi[T(x), ...] \\ & + \int \mathrm{d}x \bigg(T'(x) \frac{\delta \Psi}{\delta T(x)} + ... \bigg) \delta N^1(x). \end{aligned} \tag{47}$$

Henceforth, the momentum constraint enforces the independence of Ψ under infinitesimal coordinate transformations on the hypersurfaces. This constraint acts as a generator of infinitesimal diffeomorphisms.

2.3 Relational dynamical systems

Leibniz insisted that only observable quantities should appear in the fundamental equations. Later, Ernst Mach implied that physics should only use relational systems (Kiefer, C. (2012). Quantum Gravity).

If we are up to predicting the future of a system solely based on relative separations, the key is to introduce a 'gauge freedom' with respect to translations and rotations, and also define the choice of the time parameter τ. We suggest that the theory must be invariant under the gauge transformation

$$\mathbf{x}_k \mapsto \mathbf{x}'_k = \mathbf{x}_k + \mathbf{a}(\tau) + \boldsymbol{\alpha}(\tau)\mathbf{x}_k, \tag{48}$$

where $\boldsymbol{a}$ parametrizes translations, and $\boldsymbol{\alpha}$ parametrizes rotations. The label time can be reparametrized as

$$\tau \mapsto f(\tau), \quad \dot{f} > 0. \tag{49}$$

Equations (48) and (49) define the 'Leibniz group'. The total velocity for each particle is

$$\frac{D\mathbf{x}_k}{D\tau} := \frac{\partial \mathbf{x}_k}{\partial \tau} + \dot{\mathbf{a}}(\tau) + \dot{\boldsymbol{\alpha}}(\tau)\mathbf{x}_k. \tag{50}$$

Let us see what the terms are in equation (50). The first term on the right-hand side indicates the rate of change in some chosen frame, and the two other terms are the rate of change with respect to a τ-dependent change of frame. This velocity is not gauge invariant yet, so one might ask how can we construct a gauge invariant quantity? Such a quantity can be constructed by minimizing the 'kinetic energy' with respect to $\boldsymbol{a}$ and $\boldsymbol{\alpha}$.

This procedure is also called 'horizontal stacking'. If one is interested in grasping an intuition of how horizontal stacking works, one can imagine putting two slides with the particle positions marked on them on top of each other and moving them relative to each other until the centres of mass coincide and there is no overall rotation to be considered. The gauge-invariant velocity is called 'intrinsic velocity', that is $\mathrm{d}\mathbf{x}/\mathrm{d}\tau$. Suppose we have these velocities for each particle. If we consider a system composed of n particles, The kinematic energy is given by

$$T = \frac{1}{2}\sum_{k=1}^{n} m_k \left(\frac{\mathrm{d}\mathbf{x}_k}{\mathrm{d}\tau}\right)^2, \tag{51}$$

where m_k is the mass of each particle in the system. The potential is the standard Newtonian potential, which is

$$V = -G\sum_{k<l}\frac{m_k m_l}{r_{kl}}, \tag{52}$$

where G is the universal gravitational constant, and $r_{kl} = |x_k - x_l|$ is the relative distance.

Now one can construct the action

$$S[\mathbf{x}_k(t)] = 2\int \mathrm{d}\tau\sqrt{-VT}, \tag{53}$$

which is homogeneous in velocities and therefore is reparametrization-invariant with respect to τ (in previous sections we already demonstrated that this statement is correct). The Lagrangian is therefore $2\sqrt{-VT}$ as we can see. Using the Euler-Lagrange equation which is

$$\frac{\mathrm{d}}{\mathrm{d}\tau}\left(\frac{\partial L}{\partial \dot{\mathbf{x}}_k}\right) = \frac{\partial L}{\partial \mathbf{x}_k}, \tag{54}$$

one can write the equation of motion by using the action (53). The equation of motion is

$$\frac{\mathrm{d}}{\mathrm{d}\tau}\left(\sqrt{\frac{-V}{T}} m_k \frac{\mathrm{d}\mathbf{x}_k}{\mathrm{d}\tau}\right) = -\sqrt{\frac{T}{-V}}\frac{\partial V}{\partial \mathbf{x}_k}. \tag{55}$$

The gauge invariance with respect to translations and rotations leads to the constraints

$$\mathrm{P} = \sum_k \mathbf{p}_k = 0, \quad \mathrm{L} = \sum_k \mathbf{x}_k \times \mathbf{p}_k = 0, \tag{56}$$

that is, the total momentum and the angular momentum of the universe (if we consider all of the particles in the world) are constrained to vanish. This is clearly indicating the conservation law for these two quantities (the linear momentum, and the angular momentum).

For us to find the Hamiltonian constraint, first we write the momentum of the kth particle

$$\mathbf{p}_k = \frac{\partial L}{\partial \dot{\mathbf{x}}_k} = m_k \dot{\mathbf{x}}_k \sqrt{\frac{-V}{T}}, \tag{57}$$

then the Hamiltonian constraint can be found as

$$H \equiv \sum_{k=1}^{n} \frac{{\mathbf{p}_k}^2}{2m_k} + V = 0. \tag{58}$$

Equation (55) can be simplified by choosing a convenient gauge for τ to make the total energy vanish

$$T + V = 0. \tag{59}$$

This equation is used to define time, since there is no external time present in here. With equation (59) in our hands, we get Newton's equations from (55). Since $\sum_k E_k = 0$, the various clocks of approximately isolated subsystems march in step. To actually determine time, it is necessary to monitor the whole universe, because the only truly isolated system is the universe as a whole.

We may now consider a time-reparametrization-invariant system with no absolute time, which only relies exclusively on observational elements. The Jacobi action (a formal analogy of (53)) can be written in the form of

$$S_J[\mathbf{x}_k(t)] = 2\int_A^B \mathrm{d}t \sqrt{(E-V)T}, \tag{60}$$

where t is the Newton's absolute time and the path leads from A to B. Using (51) as the kinetic energy and

$$\mathrm{d}s^2 := \sum_{k=1}^{n} m_k \mathrm{d}\mathbf{x}_k \mathrm{d}\mathbf{x}_k, \tag{61}$$

where s parametrizes the paths, one can easily write

$$\mathrm{d}t = \frac{1}{\sqrt{2T}} \mathrm{d}s. \tag{62}$$

So the timeless form of the Jacobi action will be

$$S_J[\mathbf{x}_k(t)] = \int \mathrm{d}s \sqrt{2(E-V)}. \tag{63}$$

It is the ‘timeless’ description that employs only paths in configuration space. Speed can be determined by solving the energy equation $T + V = E$.

One can argue that for an isolated system, such as the universe, the timeless description demonstrates the redundancy of the notion of an independent time. Why is that? Because we can claim that all the essential dynamical content is already contained in the timeless paths.

3 Construction of Dirac observables

In this section, we discuss gauge transformation of the scalar field and that of the Lagrangian, covariant transformation of tensors, diffeomorphisms, defining gauge condition, constraints and Dirac observables. States should transform appropriately under gauge transformation, and observables will remain invariant under the same transformation.

Phase space functions that are gauge invariant, do not depend explicitly on spacetime coordinates, then they Poisson commute with the constraint functions. They are often called Dirac obsevables. A class of these observables is indicated by 'evolving constants of motion'. These constants can be determined as gauge-invariant extensions of non-invariant quantities given in a particular frame. What are gauge-invariant operators? They are operators that commute with the gauge generator and therefore have a physical interpretation that is independent of the time reparametrization.

In some frameworks, the physical Hilbert space can be the vector space of wave functions that are annihilated by the constraint operators. This may lead to a 'problem of time', that is when the physical states seem to be time-independent, and one could say that the dynamics is frozen. Actually the dynamics is not frozen, but rather encoded in the relational evolution of Dirac observables. A famous solution is called the 'semi-classical emergence of time': time only exists when the wave function(al) of the gravitational field is in a semi-classical regime. This interpretation is usually referred to as 'Wentzel-Kramers-Brillouin (WKB) time'. This section contents are based on [2].

3.1 Classical theory

Consider a space-time manifold as our vector space. We first define the worldline. Considering a space-time manifold, a worldline is a creature which is defined as a one-dimensional background manifold. It means that if we want to know the trajectory of a particle in spacetime, that trajectory is called a worldline. Suppose two worldline vectors $V_i = \epsilon_i(\tau)\frac{\mathrm{d}}{\mathrm{d}\tau},\ i = 1, 2$. The intrinsic metric on the worldline is given by

$$g(V_1, V_2) = e^2(\tau)\epsilon_1(\tau)\epsilon_2(\tau), \tag{64}$$

where $e(\tau)$ is a worldline scalar density called the *einbein* (by scalar, we mean its value does not change under the change of coordinates). The einbein is the induced metric, normally written as h_{ab}, where a and b range over the coordinates in the parametrization of the worldline. One is able to generate a worldline diffeomorphism by a vector field. Gauge transformations are worldline diffeomorphisms generated by a vector field $V = \epsilon(\tau)\frac{\mathrm{d}}{\mathrm{d}\tau}$. The dynamical variables are considered as worldline tensors in an arbitrary frame related to the choice of the worldline parameter τ. How do components of tensors transform under reparametrization of the worldline? They transform covariantly (the general form of a covariant transformation is $A^{i'} = \frac{\partial x^{i'}}{\partial x^j}A^j$). Hence we can define observables to be worldline tensors. We are interested in describing the initial values in a gauge-invariant manner. Then we construct Dirac observables to be: obejects that commute with the phase- space constraints, to represent the invariant extensions of initial values of worldline tensors (dynamical observables).

We assume the fundamental dynamical fields are worldline scalars. The gauge transformation of a scalar field $q(\tau)$ read

$$\delta q(\tau) := \epsilon(\tau)\frac{\mathrm{d}q}{\mathrm{d}\tau}. \tag{65}$$

Now for the dynamics to be reparametrization invariant, the Lagrangian $L\big(q(\tau), \dot{q}(\tau)\big)$ must be a worldline scalar density. Then it transforms as

$$\delta L := \frac{\mathrm{d}}{\mathrm{d}\tau}\big(\epsilon(\tau)L\big). \tag{66}$$

Using the Lagrangian, One can simply write the action as

$$S = \int_a^b \mathrm{d}\tau \; L\big(q(\tau), \dot{q}(\tau)\big). \tag{67}$$

The variation of the action is written as

$$\begin{aligned} \delta S = &\int_a^b \mathrm{d}\tau \; \delta L\big(q(\tau), \dot{q}(\tau)\big) = \int_a^b \mathrm{d}\tau \; \frac{\mathrm{d}}{\mathrm{d}\tau}\left(\epsilon(\tau)L\right) \\ &= \epsilon(\tau)L\Big|_a^b. \end{aligned} \tag{68}$$

The action is then invariant if the infinitesimal diffeomorphism $\epsilon(\tau)$ vanishes at the end points, meaning $\epsilon(a) = \epsilon(b) = 0$. Otherwise, we have to consider boundary terms for the action to make it invariant. In general, the quantity

$$O_\omega = \int_\alpha^\beta \mathrm{d}\tau \; \omega(\tau) \tag{69}$$

is invariant and hence observable (assuming that $\omega(\tau)$ transforms as in equation (66)) if the integral converges and suitable boundary terms are chosen. For example one could restrict periodic boundary conditions $\epsilon(\alpha) = \epsilon(\beta), \; \omega(\alpha) = \omega(\beta)$.

As mentioned before, an important class of observables is given by the evolving constants. First, we introduce *on-shell* tensor fields: fields which are solutions of equations of motion. Evolving constants encode the relational evolution of on-shell tensor fields. These fields can be constructed by defining a parametrization of the worldline (defining a gauge condition). Consider τ as an arbitrary initial parameter and define s as a new time coordinate. We use the equation

$$\chi\big(q(\tau), \dot{q}(\tau), e(\tau)\big) = s, \tag{70}$$

in which χ is a worldline scalar. This condition is admissible if

$$\Delta_\chi := \frac{\mathrm{d}\chi}{\mathrm{d}\tau} \neq 0. \tag{71}$$

One can solve (70) for τ to find coordinate transformation

$$\tau = \phi\big(q(0), \dot{q}(0), e(0), s\big), \tag{72}$$

where ϕ defines a field-dependent diffeomorphism on the wolrdline. Using ϕ makes us able to pull back tensor fields. The invariant extensions of initial values can then be obtained by writing the pull back in an arbitrary parametrization. As an example, we consider the Lagrangian

$$L = \frac{\dot{q}^2}{2\dot{t}}, \tag{73}$$

which is the Lagrangian of a free particle. Then we try to compute and compare the Hamiltonian for $\chi = q(\tau)$ and $\chi = t(\tau)$. For $\chi = q(\tau)$ we have

$$q = s, \quad \dot{s} \equiv (\frac{\mathrm{d}}{\mathrm{d}s})s = 1 \quad \text{then} \quad L = \frac{1}{2\dot{t}}. \tag{74}$$

The canonical momentum and the Hamiltonian will become

$$p = \frac{\partial L}{\partial \dot{t}} = -\frac{1}{2\dot{t}^2}, \quad H = \frac{\partial L}{\partial \dot{t}}\dot{t} - L = -i\sqrt{2p}. \tag{75}$$

By using the above equations, one can actually find t as a function of q (consider for example the case of a simple harmonic oscillator. What we usually do, is to find the spatial coordinate q as a function of t. But with this choice of gauge condition we made which was $\chi = q(\tau)$, we are trying to find the time t as a function of q. The physics is the same but obviously, we will end up with somewhat different equations to describe the motion for us). Now for $\chi = t(\tau)$, we compute

$$t = s \quad \text{then} \quad L = \frac{\dot{q}^2}{2}, \tag{76}$$

$$H = \frac{\partial L}{\partial \dot{q}}\dot{q} - L = \frac{\dot{q}^2}{2}, \tag{77}$$

As we can see, the choice of $t(\tau)$ gives us what we are already used to it. But when we substitute a scalar field (such as a spatial coordinate) with time, we may face somehow unfamiliar results which are strange to our usual intuitions.

The Dirac delta distribution is defined as

$$\int_{-\infty}^{\infty} \mathrm{d}\tau \; \delta(\tau) f(\tau) = f(0). \tag{78}$$

Suppose that $f(\tau)$ is a scalar field. Take equation (69) and let $\alpha \to -\infty$, $\beta \to \infty$ (we are able to allow this since the function is integrable in the interval $-\infty, \infty$). Now one could write this integral with a gauge condition as

$$\begin{aligned} O[f|\chi = s] &:= f(\tau)|_{\tau=\phi} \\ &= \int_{-\infty}^{\infty} \mathrm{d}\tau \; \delta\left(\tau - \phi(q(0), \dot{q}(0), e(0), s)\right) f(\tau) \\ &= \int_{-\infty}^{\infty} \mathrm{d}\tau \; \left|\frac{\mathrm{d}\chi}{\mathrm{d}\tau}\right| \delta(\chi(q(\tau), \dot{q}(\tau), e(\tau)) - s) f(\tau). \end{aligned} \tag{79}$$

We do suppose that equation (71) holds, and the above integral converges. For any fixed value of $s = s_0$, equation (79) defines an invariant extension of the initial value of $\phi^* f|_{s=s_0}$. These invariant extensions are Dirac observables which are independent of the choice of τ.

As a practice, let us calculate the Dirac observable associated with the identity function, that is $f(\tau) = 1$

$$\begin{aligned} O[1|\chi = s] &= \int_{-\infty}^{\infty} \mathrm{d}\tau \left|\frac{\mathrm{d}\chi}{\mathrm{d}\tau}\right| \delta(\chi(q(\tau), \dot{q}(\tau), e(\tau)) - s) \\ &= \int_{-\infty}^{\infty} \mathrm{d}\tau \ \delta(\tau - \phi(q(0), \dot{q}(0), e(0), s)) = 1. \end{aligned} \tag{80}$$

The above equation is called the 'Faddeev-Popov resolution of the identity' for the gauge condition χ. Another practice is constructing the Dirac observable associated with the gauge condition itself

$$O[\chi|\chi = s] = \int_{-\infty}^{\infty} \mathrm{d}\tau \left|\frac{\mathrm{d}\chi}{\mathrm{d}\tau}\right| \delta(\chi(q(\tau), \dot{q}(\tau), e(\tau)) - s) \chi(q(\tau), \dot{q}(\tau), e(\tau)) = s. \tag{81}$$

These integrals are gauge-invariant extensions and independent of the choice of τ, but they generally depend on the gauge condition introduced in (70). Actually, they yield gauge-invariant but not gauge-independent objects. This procedure represents the value of the scalar field f when χ has the value of s_0. In other terms, they encode the on-shell relational evolution between the scalar fields.

We shall proceed to deal with the Hamiltonian and the gauge generator. One can take the fundamental fields $q(\tau)$ to be worldline scalars, and then finds out what will happen to the Hamiltonian. To obtain the derivative of $\epsilon(\tau)L$ with respect to the time parameter τ, we should use (65) and (66). This derivative is written as

$$\begin{aligned} \frac{\mathrm{d}}{\mathrm{d}\tau}(\epsilon(\tau)L) = \delta_{\epsilon(\tau)} L &= \frac{\partial L}{\partial q^i} \delta_{\epsilon(\tau)} q^i(\tau) + \frac{\partial L}{\partial \dot{q}^i} \delta_{\epsilon(\tau)} \dot{q}^i(\tau) \\ &= \frac{\partial L}{\partial q^i} \epsilon(\tau) \dot{q}^i(\tau) + \frac{\partial L}{\partial \dot{q}^i} \epsilon(\tau) \ddot{q}^i(\tau) + \frac{\partial L}{\partial \dot{q}^i} \dot{\epsilon}(\tau) \dot{q}^i(\tau) \\ &= \frac{\mathrm{d}}{\mathrm{d}\tau}(\epsilon(\tau)L) + \dot{\epsilon}(\tau) \left(\frac{\partial L}{\partial \dot{q}^i(\tau)} \dot{q}^i(\tau) - L \right). \end{aligned} \tag{82}$$

It is obvious that the coefficient of $\dot{\epsilon}(\tau)$ which appeared in the parenthesis, is equal to zero. This result shows that the Hamiltonian vanishes as

$$H(q(\tau), p(\tau)) = p_i(\tau) \dot{q}^i(\tau) - L(q(\tau), \dot{q}(\tau)) = 0, \tag{83}$$

where the momenta are defined in their usual way. Another result which equation (83) implies, is that the Lagrangian is singular:

$$\frac{\partial^2 L}{\partial \dot{q}^i \partial \dot{q}^j} \dot{q}^j = 0. \tag{84}$$

This means that we can't invert $p_i(\tau) = \partial L/\partial \dot{q}^i$ to find the velocities as the functions of coordinates and momenta. In other words, the momenta are not independent and are generally related by the constraints $C(q,p) = 0$.

Assume there is only one constraint. The constraint $C(q,p) = 0$ defines a surface in the phase space. In general, these surfaces can be defined by $f(c) = 0$. To describe the dynamics of the system in the phase space, one must impose restrictions on the constraint functions which are known as 'regularity conditions'. For the simple case, the regularity conditoions lead to require the constraint surfaces to be coverable by open regions. This statement means that the differential of $C(q,p)$ must not be equal to zero on the constraint surface, which is written as

$$\frac{\partial C}{\partial q^i}\mathrm{d}q^i + \frac{\partial C}{\partial p_i}\mathrm{d}p_i \neq 0. \tag{85}$$

In the following approach, we assume that the constraint surface is defined by a function $C(q,p)$ which satisfies (85) on the constraint surface. Equation (83) gives us $H \approx 0$, since the canonical Hamiltonian is well defined only if $C(q,p) = 0$. This allows us to define an arbitrary parameter λ which is an worldline scalar density. We may write

$$H = \lambda(\tau; q(\tau), p(\tau))C(q(\tau), p(\tau)). \tag{86}$$

As we already know, the choice of einbein $e(\tau; q(\tau), p(\tau))$ is also arbitrary. Then we may choose $e(\tau; q(\tau), p(\tau)) = \lambda(\tau; q(\tau), p(\tau))$, to obtain

$$H = e(\tau; q(\tau), p(\tau))C(q(\tau), p(\tau)). \tag{87}$$

Consider a phase-space function $g(\tau; q(\tau), p(\tau))$. The evolution in time of this function is determined by

$$\frac{\mathrm{d}g}{\mathrm{d}\tau} = \frac{\partial g}{\partial \tau} + \{g, eC\} \approx \frac{\partial g}{\partial \tau} + e\{g, C\}, \tag{88}$$

where the Poisson bracket is

$$\{g, H\} = \frac{\partial g}{\partial q^i}\frac{\partial H}{\partial p_i} - \frac{\partial H}{\partial q^i}\frac{\partial g}{\partial p_i}. \tag{89}$$

There is a rather crucial question that one might ask here, which is: Can gauge transformations be represented as canonical transformations in phase space? consider a worldline scalar $f(q(\tau), p(\tau))$ with no explicit τ dependence. We have

$$\delta_{\epsilon(\tau)}f = \epsilon(\tau)\frac{\mathrm{d}f}{\mathrm{d}\tau} = \epsilon(\tau)\{f, eC\} \approx \{f, \epsilon(\tau)eC\} =: \{f, G\}. \tag{90}$$

then, the reparametrizations of such worldline scalars are on-shell canonical transformations generated by

$$G(\tau; q(\tau), p(\tau)) = \epsilon(\tau)e(\tau; q(\tau), p(\tau))C(q(\tau), p(\tau)), \tag{91}$$

which is called the 'gauge generator'.

We already stated that equation (79) describes a quantity which is an invariant extension of $\phi^* f$ for each value of $s = s_0$. It is actually independent of the choice of initial arbitrary parameter τ. It defines a Dirac observable, and it Poisson commutes with the gauge generator. The phase-space constraint generates evolution in *proper time*, defined as

$$\eta := \int \mathrm{d}\tau \; e(\tau). \tag{92}$$

We would like to write (79) in terms of the proper time. Once more we consider g as a phase-space function with no explicit time dependence. One may obtain

$$\{g, C\} \approx \frac{1}{e}\{g, H\} = \frac{1}{e}\frac{\mathrm{d}g}{\mathrm{d}\tau} =: \frac{\mathrm{d}g}{\mathrm{d}\eta}, \tag{93}$$

then equation (79) can be written as

$$\begin{aligned} O[f|\chi = s_0] &= \int_{-\infty}^{\infty} \mathrm{d}\eta \left|\frac{\mathrm{d}\chi}{\mathrm{d}\eta}\right| \delta(\chi(q(\eta), p(\eta)) - s_0) f(q(\eta), p(\eta)) \\ &\equiv \int_{-\infty}^{\infty} \mathrm{d}\eta \; \omega[f|\chi = s_0], \end{aligned} \tag{94}$$

which is valid only if we assume that both f and χ have no explicit time dependence. From (93) and (94), we can write

$$\{O[f|\chi = s_0], C\} \approx \int_{-\infty}^{\infty} \mathrm{d}\eta \; \frac{\mathrm{d}}{\mathrm{d}\eta}\omega[f|\chi = s_0] = 0. \tag{95}$$

This result is acceptable if

$$\lim_{|\eta| \to \infty} \omega[f|\chi = s_0] = 0, \tag{96}$$

is true for the initial values of s_0, and initial conditions $q(0), p(0)$.

In the following paragraphs, we are about to discover how one is supposed to consider dynamics for the Dirac observables which have been discussed already. If one wants to know how the pullback is done for a on-shell scalar function $f(q(\tau), p(\tau))$, using equation (72) would give the appropriate relation between τ and $\phi(s)$. As written in (79), one can rewrite

$$\begin{aligned} \frac{\mathrm{d}}{\mathrm{d}s} O[f|\chi = s] &= \frac{\mathrm{d}}{\mathrm{d}s} f(q(\phi(s)), p(\phi(s))) \\ &= \frac{\mathrm{d}\phi}{\mathrm{d}s}\left[\frac{\mathrm{d}f}{\mathrm{d}\tau}\right]_{\tau=\phi} \\ &= \frac{\mathrm{d}\phi}{\mathrm{d}s}\{f, H\}_{\tau=\phi}. \end{aligned} \tag{97}$$

The derivatives of f are taken with respect to the original set of fields, which are $q(\tau)$ and $p(\tau)$. At the end, one can set $\tau = \phi(s)$. Since equation (71) holds, by setting $f = \chi$ we can get

$$\frac{\mathrm{d}\phi}{\mathrm{d}s} = \frac{1}{\{\chi, H\}_{\tau=\phi(s)}}. \tag{98}$$

We are already familiar with the lapse function. Equation (98) gives us the rate of the change of the time parameter with respect to the new time coordinate s. Therefore, it is a gauge-fixed lapse function. If we insert (98) in (97), we get

$$\frac{\mathrm{d}}{\mathrm{d}s}O[f|\chi = s] = \frac{1}{\{\chi, H\}_{\tau=\phi(s)}}\{f, H\}_{\tau=\phi}, \tag{99}$$

which leads us to the understanding that the dynamics of observables is not frozen in general. Actually, the above equation gives us the gauge-fixed equations of motion for dynamical variables.

3.2 Quantum theory

In the previous section, we discussed and tried to construct some aspects of the general framework of Dirac observables. Observables, Hamiltonian, gauge generators, evolving constants as invariant extensions, and the dynamics of Dirac observables were the main subjects which have been talked about in the classical manner of physics.

Now we are about to introduce the physical Hilbert space and the operators which are normally used in quantum mechanics. Assume the classical phase-space constraint $C(q,p)$. We promote this constraint to a linear operator $\hat{C}$, and it is self-adjoint in an auxiliary Hilbert space of square-integrable functions equipped with an auxiliary inner product. One can understand that in this way, $\hat{C}$ has a complete orthogonal system of eigenstates. Its eigenvalue is the energy of the system.

$$\hat{C}\ |E, \mathbf{k}\rangle = E\ |E, \mathbf{k}\rangle, \tag{100}$$

$$\langle E', \mathbf{k}'|E, \mathbf{k}\rangle = \delta(E', E)\delta(\mathbf{k}', \mathbf{k}), \tag{101}$$

where $\mathbf{k}$ labels the degeneracies here. The δ symbol here can be considered both a Kronecker or a Dirac delta depending on the spectrum of $\hat{C}$. If the spectrum is discrete, it is the Kronecker delta, and if it is continuous, it is the Dirac delta. One may ask: What is the analogue of the classical constraint surface $C(q,p)$? It is the linear subspace of states in the kernel of $\hat{C}$, which can be written as superpositions of $|E = 0, \mathbf{k}\rangle$ (what is a kernel? Consider two vector spaces V and W. assume L as the linear map between these vector spaces, that is $L : V \to W$. The kernel of L is the vector space of all elements $\boldsymbol{v}$ of V such that $L(\boldsymbol{v}) = 0$, where 0 denotes the zero vector in W). The overlap of these states reads

$$\langle E = 0, \mathrm{k}'|E = 0, \mathrm{k}\rangle = \delta(0, 0)\delta(\mathrm{k}', \mathrm{k}). \tag{102}$$

If zero is in the continuous part of the spectrum of $\hat{C}$, the factor of $\delta(0,0)$ is divergent. Then the auxiliary inner product cannot be used in this subspace. Therefore we define a regularized inner product on the kernel of $\hat{C}$, such that

$$\langle E', \mathrm{k}'|E, \mathrm{k}\rangle =: \delta(E', E)(E', \mathrm{k}'|E, \mathrm{k}), \tag{103}$$

$$(E = 0, \mathrm{k}'|E = 0, \mathrm{k}) = \delta(\mathrm{k}', \mathrm{k}). \tag{104}$$

Now we consider the superpositions

$$|\phi_E^i\rangle = \sum_{\mathrm{k}} \phi^i(\mathrm{k})|E,\mathrm{k}\rangle, \quad i = 1, 2. \tag{105}$$

If the degeneracies are labeled by continuous indices, one may replace the sum by an integral. By using (104), we are able to write the inner product for general invariant states

$$(\phi_{E=0}^{(1)}|\phi_{E=0}^{(2)}) = \sum_{\mathrm{k}} \bar{\phi}^{(1)}(\mathrm{k})\phi^{(2)}(\mathrm{k}). \tag{106}$$

With the above equation in our hands, we are finally ready to define the physical Hilbert space for our theory: The kernel of $\hat{C}$ equipped with the inner product (106).

Now it is the time for us to attempt constructing an operator which corresponds to the classical Dirac observables. First, we shall define the Hamiltonian operator. Using (87), the Hamiltonian operator can be written as $\hat{H} = e(\tau)\hat{C}$. The einbein $e(\tau)$ here is not a function of canonical variables, and therefore it is a c-number in the quantum theory (a c-number refers to the real numbers, and the complex numbers. Operators are called q-number in quantum mechanics). The simplest choice for the einbein is the proper time gauge, that is $e(\tau) = 1$. Suppose $\hat{A}$ is an operator. To consider time evolution for an operator (Heisenberg picture), one could write

$$\hat{A}(t) = e^{\frac{i}{\hbar}\hat{H}t}\hat{A}\ e^{-\frac{i}{\hbar}\hat{H}t}, \tag{107}$$

then according to the above equation and equation (69), the Dirac observable operator will be given by

$$\hat{O}_\omega = \int_\alpha^\beta \mathrm{d}\tau\ e^{\frac{i}{\hbar}\hat{C}\tau}\hat{\omega}\ e^{-\frac{i}{\hbar}\hat{C}\tau}. \tag{108}$$

If the spectrum of $\hat{C}$ is discrete, one can set $\alpha = 0$ and $\beta = 2\pi$, whereas if the spectrum is continuous, one would let $\alpha \to -\infty$ and $\beta \to \infty$. The matrix elements of the Dirac observable operator are

$$\langle\phi_{E'}^{(1)}|\hat{O}_\omega|\phi_E^{(2)}\rangle = 2\pi\hbar\delta(E', E)\sum_{\mathrm{k}',\mathrm{k}} \bar{\phi}^{(1)}(\mathrm{k}')\ \langle E',\mathrm{k}'|\hat{\omega}|E,\mathrm{k}\rangle\ \phi^{(2)}(\mathrm{k}), \tag{109}$$

and the regularized matrix elements are given by

$$\frac{1}{2\pi\hbar}(\phi_{E=0}^{(1)}|\hat{O}_\omega|\phi_{E=0}^{(2)}) := \sum_{\mathrm{k}',\mathrm{k}} \bar{\phi}^{(1)}(\mathrm{k}')\ \langle E=0,\mathrm{k}'|\hat{\omega}|E=0,\mathrm{k}\rangle\ \phi^{(2)}(\mathrm{k}). \tag{110}$$

Similar to the previous section, we are interested in defining the invariant extensions of initial values using the gauge condition. Therefore we define an operator $\hat{\omega}[f|\chi = s]$, such that

$$\hat{O}[f|\chi = s] = \int_{-\infty}^{\infty} \mathrm{d}\tau\ e^{\frac{i}{\hbar}\hat{C}\tau}\hat{\omega}[f|\chi = s]\ e^{-\frac{i}{\hbar}\hat{C}\tau}. \tag{111}$$

It is actually the symmetric quantization of the classical scalar Dirac observable, which was given by (79). One would particularly be interested to know that how an operator version of the Faddeev-Popov resolution of identity (80) looks like. Consider (106), we would get

$$(\phi^{(1)}_{E=0}|\hat{O}[1|\chi = s]|\phi^{(2)}_{E=0}) = \sum_{\mathrm{k}} \bar{\phi}^{(1)}(\mathrm{k})\phi^{(2)}(\mathrm{k}), \tag{112}$$

which tells us that the operator $\hat{\omega}[1|\chi = s]$, must satisfy the relation (take a look at the equation (110))

$$2\pi\hbar\langle E = 0, \mathrm{k}'|\hat{\omega}[1|\chi = s]|E = 0, \mathrm{k}\rangle = \delta(\mathrm{k}', \mathrm{k}). \tag{113}$$

The above equation holds for all values of s.

4 Quantization of a Friedmann universe

When it comes to the problem of quantizing the gravitational field, one may face many different approaches which have appeared in recent decades. One of the most interesting and satisfying approaches is the 'quantum cosmology'. The basic idea behind this approach is to freeze out all but a finite number of degrees of freedom of the system, and then quantize the remaining ones. To understand the significance of this approach, we shall point out that this significance lies in two directions: (1) Restricting the system to a finite number of degrees of freedom, makes us able to focus on the problems of quantum gravity which are peculiar to the gravitational field. Particularly, the phenomenon of gravitational collapse and the influence upon it of quantum effects can be sensibly discussed in this framework. (2) One can regard this approach as a perturbation scheme in which the perturbation is not in terms of coupling constants, but rather in terms of the number of modes quantized.

It seems pretty reasonable if we describe the matter quantum mechanically, and the simplest way to do this is to use a quantum field. Therefore we discuss the problem of a scalar matter field coupled to a Robertson-Walker metric in which both are quantized in the quantum-model sense. If such a system is quantized in the semiclassical sense of choosing the expectation value of the energy-momentum tensor of the quantized matter as the source of the classical gravitational field, then the system will not collapse but rather has a minimum radius of the Compton wavelength of the particles described in the scalar field. In this section, we are going to consider the massless case. One may face some difficulties in these types of models of a square-root, time-dependent Hamiltonian which are treated in a way that seems to be a little uncertain. The usual resolution of a square-root problem is to use a Klein-Gordon equation instead of a Schrodinger equation. However, these two are equivalent in the case where the Hamiltonian is time-dependent, therefore we may use the original Schrodinger equation and define the square-root via the spectral theorem (In mathematics, particularly linear algebra and functional analysis, a spectral theorem is a result about when a linear operator or matrix can be diagonalized). The present two-mode system can be made to look like almost any other two-mode system (in particular, some purely gravitational ones), by using a series of canonical transformations. However, quantum mechanics frequently does not respect the canonical transformations. In this section we follow [3], and also use the concepts mentioned in [1].

4.1 The classical theory

Now we shall write down the homogeneous and isotropic Robertson-walker metric to define the geometry which we are interested in

$$\mathrm{d}s^2 = N(t)^2\mathrm{d}t^2 - R(t)^2 S_{ij}\mathrm{d}x^i\mathrm{d}x^j, \tag{114}$$

where S_{ij} is the metric for a three-space of constant curvature K, and $N(t)$ is the lapse function. The curvature may have different values: $K = 1$, $K = 0$, and $K = -1$ are corresponding to the three-sphere, flat, and hyperbolic surfaces respectively. Such kind of space-time will lead to a non-vanishing Einstein tensor $G_{\mu\nu}$ and therefore it demands a source of gravitational field which is matter. The massive scalar field which we are talking about, can be given by the following Lagrangian

$$L = \frac{1}{2} g^{\frac{1}{2}} \left(g^{\mu\nu} \partial_\mu \phi \ \partial_\nu \phi - m^2 \phi^2 \right). \tag{115}$$

In the above equation, ϕ is the scalar field, and $g^{\mu\nu}$ is the metric in (114). The corresponding energy-momentum tensor is given by

$$T_{\mu\nu} = \partial_\mu \phi \ \partial_\nu \phi - \frac{1}{2} g_{\mu\nu} \left(g^{\alpha\beta} \partial_\alpha \phi \ \partial_\beta \phi - m^2 \phi^2 \right). \tag{116}$$

In order to maintain the Robertson-Walker form of the metric, since it is a homogeneous Friedmann model, we must take the scalar field to be homogeneous $\phi = \phi(t)$ (independent of spatial coordinates). Now we are beeing left with three coupled variables, which are: $N(t)$, $R(t)$ and $\phi(t)$. At this point we write down the resulting equations of motion (considering the units in which the velocity of light c and the gravitational constant G are related by $8\pi G/c^4 = \frac{1}{2}$). $G_{\mu\nu}$ is the Einstein tensor that can be obtained by the equation

$$G_{\mu\nu} = R_{\mu\nu} - \frac{1}{2} R g_{\mu\nu}, \tag{117}$$

where $R_{\mu\nu}$ is the Ricci curvature tensor. Using the Einstein field equations which are given by

$$G_{\mu\nu} + \Lambda g_{\mu\nu} = \kappa T_{\mu\nu}, \tag{118}$$

where κ is the Einstein gravitational constant, one can write the 'G_{00} equation' as (take a look at the metric and the energy-momentum tensor which are already defined)

$$3\frac{\dot{R}^2}{R^2} + \frac{3KN^2}{R^2} = \frac{1}{4}\left(\dot{\phi}^2 + m^2 N^2 \phi^2 \right). \tag{119}$$

The 'G_{ij} equation' is

$$\frac{2\ddot{R}}{R} + \frac{\dot{R}^2}{R^2} - 2\frac{\dot{R}}{R}\frac{\dot{N}}{N} + \frac{KN^2}{R^2} = \frac{1}{4}\left(-\dot{\phi}^2 + m^2 N^2 \phi^2 \right), \tag{120}$$

in which dots denote the derivative with respect to time. The Klein-Gordon equation of the scalar field ϕ is written as

$$\frac{\mathrm{d}}{\mathrm{d}t} \frac{(R^3 \dot{\phi})}{N} + m^2 \left(N R^3 \phi \right) = 0. \tag{121}$$

Before we can solve the above equations classically, a choice of time must be made. We can consider the case in which the time variable is provided by choosing $N = R$. As mentioned before, for simplicity, we also consider the massless case where $m = 0$. In this case, one can easily see that from the Klein-Gordon equation we have $R^3\dot{\phi}/N$ as a constant of motion. Then the equations (119) and (120) can be solved to give us R and ϕ as (in the $K > 0$)

$$R^2(t) = {R_m}^2 \sin\left(2\sqrt{K}t + \delta\right), \tag{122}$$

$$\phi(t) = \phi_0 + \sqrt{3}\ln\left[\tan\left(\sqrt{K}t + \frac{1}{2}\delta\right)\right], \tag{123}$$

where R_m, ϕ_0 and δ are constants. From the above equations it is clear that for a positive-curvature case, there is a maximum radius of expansion R_m, and also the system experiences gravitational collapse. The solution for the negative-curvature $K < 0$ can be obtained the same way as the other case from equations (119) and (120). In this case also there is a gravitational collapse phenomenon, but there is no maximum value for the radius parameter anymore. The parameter δ is an additive constant in the definition of time, henceforth it is arbitrary and one can set it equal to zero for the sake of more convenience.

Now let us discuss the different values of $\phi - \phi_0$ according to (123) which are in the range of $-\infty$ to ∞. For example, consider these amounts of time t below:

$$\begin{aligned}
&\text{if} \quad t = 0 \quad \text{then} \quad \phi - \phi_0 = -\infty, \\
&\text{if} \quad t = \frac{\pi}{4\sqrt{K}} \quad \text{then} \quad \phi - \phi_0 = 0, \\
&\text{if} \quad t = \frac{\pi}{2\sqrt{K}} \quad \text{then} \quad \phi - \phi_0 = +\infty.
\end{aligned}$$

At $t = \frac{\pi}{4\sqrt{K}}$, we have $R = R_m$ which corresponds to the maximum expansion. It is obvious that at this point, $\phi - \phi_0$ changes sign.

One can use equations (122) and (123) to eliminate the parameter t, and therefore achieve the following relation

$$\phi(R) - \phi_0 = \mp\sqrt{3}\ln\frac{R_m^2 + \left(R_m^4 - R^4\right)^{\frac{1}{2}}}{R_m^2 - \left(R_m^4 - R^4\right)^{\frac{1}{2}}}, \tag{124}$$

where the negative and positive signs describe expansion and contraction phases respectively. Equivalently in terms of R, we have

$$R(\phi) = \frac{R_m}{\cosh^{\frac{1}{2}}\left[(\phi - \phi_0)/2\sqrt{3}\right]}. \tag{125}$$

It may come in handy to know the equation for R in the case where the space is flat which corresponds to $K = 0$. This equation is

$$R(\phi) = R_0 e^{\pm(\phi-\phi_0)/2\sqrt{3}}. \tag{126}$$

These equations we mentioned, describe the intrinsic dynamics of the system expressed in terms of the correlation between ϕ and R, and are independent of the choice of time.

We are interested in canonical quantization. So our goal will be constructing a set of genuine canonical variables whose first-order equations of motion are equivalent to equations (119)-(121). The equations which contain variables that eliminate by a choice of time, are not genuine dynamical ones. One solution to this problem is to fix the parameter which is representing time, to eliminate the redundant values from our equations. Let us consider the canonical moments π_ϕ, π_R and π_N. These moments are cojugates to ϕ, R and N respectively. The covariance of the equations of motion manifests itself by the G_{00} eqaution (119). They will appear as a constraint among these variables (R, ϕ and N). Since there is no $\dot{N}$ in the G_{00} equation, we must consider an additional constraint which is $\pi_N = 0$. The main obstacle to quantization is the existence of these constraint equations.

There is another approach that was developed from the work of Paul Dirac. In this approach, the G_{00} constraint is still there, but the difference is that the constraint $\pi_N = 0$ is replaced by another statement, which is: N variable is simply considered as a Lagrangian multiplier. Now we state the result that can be derived from the system of the equations above using the first order Lagrangian

$$L(t) = \pi_R \dot{R} + \pi_\phi \dot{\phi} + N\left(\frac{\pi_R^2}{24R} + 6KR - R^3\phi^2\frac{m^2}{2} - \frac{\pi_\phi^2}{2R^3}\right), \tag{127}$$

in which the variables π_R, R, π_ϕ, ϕ, and N must be varied independently. What exactly is this Lagrangian we just stated? It is the usual Lagrangian for the general relativity with the matter Lagrangian equation (115) added on. This Lagrangian demonstrates the role of N as a Lagrangian multiplier obviously. Actually, one can obtain the G_{00} equation by varying N. The main purpose of introducing this Lagrangian is that it makes us able to reduce the system to a true canonical form after any choice of time that we are willing to make.

The parenthesis in equation (127) can be regarded as the 'super Hamiltonian' H_s, and therefore one may quantize the superspace by substituting $\pi_R \to -i\hbar\partial/\partial R$, $\pi_\phi \to -i\hbar\partial/\partial\phi$, and considering the classical G_{00} equation ($H = 0$) as in the form of $\hat{H}\psi = 0$. However, what we are interested to do is reducing the system to a true canonical form and then starting the quantization process. This means that we gotta solve the constraint equation $H = 0$ classically, then make a choice of time, and finally substitute the result in the Lagrangian (remember that these two steps are not independent actually). For example, let us choose $t = R$ which is the simplest 'intrinsic' time. The intrinsic time is defined as the time expressed in terms of intrinsic geometry. Now we shall solve the constraint equation which is

$$\frac{\pi_R^2}{24R} + 6KR - R^3\phi^2\frac{m^2}{2} - \frac{\pi_\phi^2}{2R^3} = 0. \tag{128}$$

We solve the above equation for π_R, then substituting it in the Lagrangian leaves us with

$$L = \pi_\phi \dot{\phi} \pm (24t)^{\frac{1}{2}} \left(-6Kt + t^3 \phi^2 \frac{m^2}{2} + \frac{\pi_\phi^2}{2t^3} \right)^{\frac{1}{2}}, \tag{129}$$

which indicates that the (positive) Hamiltonian is written as

$$H = (24t)^{\frac{1}{2}} \left(-6Kt + t^3 \phi^2 \frac{m^2}{2} + \frac{\pi_\phi^2}{2t^3} \right)^{\frac{1}{2}}. \tag{130}$$

Obviously, the $t = R$ case is only appropriate for an expanding system (this expansion is with respect to the local proper time). Practically, one can redefine time at the point of maximum R in order to keep a positive Hamiltonian. In the following section, which is about quantization, we will take a look at other possible times of interest.

4.2 Quantization of the model

We already stated that we are interested in reducing the equations of motion to a true canonical form. At this point, one must define the Hilbert space. The Hilbert space will be square-integrable functions defined on the classical configuration space (the L^2 space). The quantum Hamiltonian operator is constructed from canonical operators, and the time-dependent Schrodinger equation should be solved. However, there is a problem which one faces here: The Hamiltonian is typically of square-root, and it is in addition time-dependent (take a look at the equation (130)).

The time-dependent Schrodinger equation with x as the configuration variable and p as it's conjugate momentum is written as

$$H(\hat{x}, \hat{p}, t)\ \psi(x,t) = i\hbar \frac{\partial \psi(x,t)}{\partial t}. \tag{131}$$

Note that the time t here is not an operator, and it is merely a parameter. Because of the square-root form of H, it would be nice to use the Klein-Gordon equation instead of the the Schrodinger equation

$$H^2(t)\ \psi(x,t) = -\hbar^2 \frac{\partial^2 \psi}{\partial t^2}, \tag{132}$$

where we have dropped x and p in the Hamiltonian for convenience. The above equation actually gives the time evolution of an allowed state vector. One may want to define the square-root itself. That is possible by using the spectral theorem: The operator whose square-root is being constructed, is a genuine positive self-adjoint operator which acts on the Hilbert space.

Now let us consider the integration of equation (132) which is given by

$$\psi(x,t) = e^{-\frac{i}{\hbar} H(t-t_0)} \psi(x,t_0). \tag{133}$$

This equation is not correct since the Hamiltonian is time-dependent. The problem is that the exponential of an integral of an operator, contains commutators of the operator at different times (due to the Baker-Campbell-Hausdorff formula). Since, in general, the H does not commute with itself at different times, The correct form is

$$\psi(x,t) = T\Bigg[\exp\bigg(-\frac{i}{\hbar}\int_{t_0}^{t} H(s)\mathrm{d}s\bigg)\Bigg]\psi(x,t_0), \tag{134}$$

where T is the Dyson time-ordering symbol, and s is a new time coordinate. However, If the Hamiltonian at different times commute

$$[H(s), H(s')] = 0, \tag{135}$$

then the time-ordering operation can be neglected, and equation (134) can be simply written as

$$\psi(x,t) = \Bigg[\exp\bigg(-\frac{i}{\hbar}\int_{t_0}^{t} H(s)\mathrm{d}s\bigg)\Bigg]\psi(x,t_0). \tag{136}$$

There is also another consequence which can be derived from equation (135). It actually makes it possible to find a complete set of basis states which are simultaneous eigenstates of the energy at all times. Consider $\psi_E(x)$ as an eigenstate of $H(t_0)$ at some time t_0. We have

$$H(t_0)\psi_E(x) = E\ \psi_E(x). \tag{137}$$

There exists $E(t)$ with $E(t_0) = E$, such that

$$H(t)\psi_E(x) = E(t)\psi_E(x). \tag{138}$$

Now if we want to describe the time evolution of $\psi_E(x)$, we use

$$\psi(x,t) = \Bigg[\exp\bigg(-\frac{i}{\hbar}\int_{t_0}^{t} E(s)\mathrm{d}s\bigg)\Bigg]\psi(x,t_0). \tag{139}$$

The above equation leaves us with the complete solution to the time evolution problem, which is what we needed.

Let us proceed to the discussion of the choice of time and how it works for all the things that we have talked about. We reconsider the equation (130) (in which we had $t = R$ situation). Classically we have

$$H = \sqrt{24}\bigg(-6Kt^2 + t^4\phi^2\frac{m^2}{2} + \frac{\pi_\phi^2}{2t^2}\bigg)^{\frac{1}{2}}. \tag{140}$$

We need to know about the Hilbert space for our quantization purpose. The Hilbert space here is $L^2(-\infty,\infty)$, and there are some assignments associated with this space, which are

$$(\hat{\phi}\psi)(\phi) = \phi\ \psi(\phi), \tag{141}$$

$$(\hat{\pi}_\phi \psi)(\phi) = -i\hbar \frac{\mathrm{d}\psi}{\mathrm{d}\phi}(\phi), \tag{142}$$

that obviously lead to self-adjoint operators. One can see that in equation (140), the quantity in parenthesis will be positive for t, only if we have $K \leq 0$. It means that only in flat or hyperbolic surfaces this choice of time will be appropriate. However, also for a suitable range of t it (the quantity in parenthesis) can be positive despite having the curvature constant appear as $K > 0$. For non-zero masses in equation (140), one obtains $[H(s), H(s')] \neq 0$ which leads to complicated time evolution problems. Therefore, we consider only the massless case. Now that equation (135) holds, we can use equations (136) and (139) which give us the evolution techniques. Let us solve the energy eigenvalue equation, that is

$$\hat{H}(t_0)\psi_E(\phi) = E\psi_E(\phi). \tag{143}$$

It is more convenient if we eliminate the square-root by using

$$H^2(t_0)\psi(\phi) = E^2\psi(\phi). \tag{144}$$

Now by considering equations (141) and (142), we square the Hamiltonian in (140) (put $m = 0$. What is there to say about $H^2(t)$? It is a self-adjoint operator on L^2 Hilbert space that has a continuous spectrum $(-144t^2K, \infty)$). This procedure leaves us with the following equation which can be easily solved for eigenstates $\psi_E(\phi)$:

$$\frac{\mathrm{d}^2\psi_E}{\mathrm{d}\phi^2} + \frac{t_0^2}{12\hbar^2}\left(E^2 + 144t_0^2K\right)\psi_E(\phi) = 0. \tag{145}$$

The above equation looks just like the equation for a SHO (simple harmonic oscillator). The general solution for such a equation can be written as

$$\psi_E(\phi) = ae^{i\lambda\phi} + be^{-i\lambda\phi}, \tag{146}$$

where λ parameter is given by

$$\lambda^2 = \frac{t_0^2}{12\hbar^2}(E^2 + 144t_0^2K) \geq 0. \tag{147}$$

These eigenfunctions are also the eigenfunctions of $H(t)$ with eigenvalue $E(t)$.

If we want to have the time evolution for these eigenfunctions, we shall use equation (139) to write

$$\begin{aligned}\psi(x,t) &= \left[\exp\left(-\frac{i}{\hbar}\int_{t_0}^{t} E(s)\mathrm{d}s\right)\right]\psi(x,t_0)\\ &= \left[\exp\left(-\frac{i}{\hbar}\int_{t_0}^{t}\frac{1}{s}\left[t_0^2\left(E^2 + 144t_0^2K\right) - 144Ks^4\right]^{\frac{1}{2}}\ \mathrm{d}s\right)\right]\psi(x,t_0).\end{aligned} \tag{148}$$

There is a time called the 'Misner's exponential time' which is $\Omega = -\ln R$. One could use this kind of time instead of R itself to change the spectrum from $(0, \infty)$ to $(-\infty, \infty)$.

Now let us proceed to another choice of time which is conjugate to the one we already discussed ($t = R$). This definition is written as $t = \pi_R$, that is a simple example of an extrinsic time. What is the difference between being intrinsic and being extrinsic? Well, extrinsic time is not expressed in terms of the intrinsic geometric properties, while $t = R$ is an obvious case where the time we defined is actually behaving as a part of intrinsic geometry. This new time variable $t = \pi_R$ has the advantage to describe the case in which $K > 0$ (that makes us able to cover the point of maximum expansion). The $\pi_R \in (-\infty, 0)$ is the expansion phase, and $\pi_R \in (0, \infty)$ is the contraction phase. Remember the constraint equation (128). This equation must be solved for R, and after substituting R in the Lagrangian (129), the Hamiltonian will appear as

$$H^2 = \frac{-\frac{1}{12}t^2 \pm \left(\frac{1}{144}t^4 + 48K\pi_\phi^2\right)^{\frac{1}{2}}}{24K}. \tag{149}$$

This Hamiltonian is obviously the most appropriate one for the positive curvature ($K > 0$) case. Choosing the plus sign leaves us with a positive self-adjoint operator. In this case ($t = \pi_R$) too, the Hamiltonian commutes at different times ($[H(s'), H(s)] = 0$) so we are allowed to proceed as we did for the previous case. So again we consider

$$H^2(t_0)\psi_E(\phi) = E^2\psi_E(\phi). \tag{150}$$

Using again the equations (141) and (142), leads us to the equation which will be solved for states

$$\frac{\mathrm{d}^2\psi_E}{\mathrm{d}\phi^2} + \frac{E^2}{12\hbar^2}\left(t_0^2 + 144E^2K\right)\psi_E = 0. \tag{151}$$

The eigenfunction ψ_E has the general form

$$\psi_E(\phi) = ae^{i\lambda\phi} + be^{-i\lambda\phi}, \tag{152}$$

with

$$\lambda^2 = \frac{E^2}{12\hbar^2}\left(t_0^2 + 144E^2K\right). \tag{153}$$

Let us take a look at the equations (151) and (153). One could obtain these equations from (145) and (147) respectively, by simply substituting t_0 with E. This result is not unexpected since the latter choice of time is the conjugate of the former one.

We would like to consider the case of another type of time, which is called 'the York time'. This kind of time is expressed in terms of the matter field ϕ itself. We are already familiar with the next steps: put $t = \phi$, solve (128) for π_ϕ, substitute π_ϕ in the Lagrangian, and finally we get the Hamiltonian we need. The Hamiltonian is

$$H^2 = \frac{1}{12}R^2\pi_R^2 + 12KR^4 - R^6t^2m^2. \tag{154}$$

We can see at a glance that this Hamiltonian is time-independent for a massless case. Just like the situation with $t = \pi_R$, this type of time has the advantage to describe both expansion and collapse phases. We use $L^2(0, \infty)$ as our Hilbert space in quantum theory, because the range of R values is $(0, \infty)$. One may think, as usual, the assignments are

$$R \to R, \quad \pi_R \to -i\hbar \frac{\mathrm{d}}{\mathrm{d}R}. \tag{155}$$

But these assignments are not going to work. Because the second one corresponds to a non-self-adjoint operator. Actually the symmetric operator $-i\frac{\mathrm{d}}{\mathrm{d}R}$ has no self-adjoint extensions in this Hilbert space. One can make this problem go away by changing the Hilbert space to $L^2(-\infty, \infty)$. However, this problem can be solved more directly without having the Hilbert space changed. We can make some substitutions to make a self-adjoint form for the operator H^2, even if these assignments are not self-adjoint themselves. The momentum operator π_R can be defined in a way to become a true self-adjoint operator. One can indicate that an operator like $\hat{O} \equiv -(\mathrm{d}/\mathrm{d}R)R^2\mathrm{d}/\mathrm{d}R$ is a positive self-adjoint operator in $L^2(0, \infty)$ Hilbert space. Henceforth, we define the momentum to be

$$\hat{\pi}_R \equiv \frac{1}{R}\sqrt{\hat{O}}. \tag{156}$$

The case here is $K > 0$, and thus here the H^2 is a positive self-adjoint operator whose positive square-root H does actually exist. Now let us substitute the above assignment (equation (156)) in H^2 to get

$$H^2 = -\frac{\hbar^2}{12}\frac{\mathrm{d}}{\mathrm{d}R}R^2\frac{\mathrm{d}}{\mathrm{d}R} + 12KR^4, \tag{157}$$

where the mass is set equal to zero. The familiar energy eigenfunction equation is

$$H^2\psi_E(R) = E^2\psi_E(R). \tag{158}$$

We easily substitute H^2 in the above equation to get the equation for $\psi_E(R)$, which is

$$\frac{\mathrm{d}^2\psi_E}{\mathrm{d}R^2} + \frac{2}{R}\frac{\mathrm{d}\psi_E}{\mathrm{d}R} + \frac{12}{\hbar^2}\left(\frac{E^2}{R^2} - 12KR^2\right)\psi_E = 0. \tag{159}$$

If one is interested in the general solution for the above equation, it is given in [3].

It is interesting to know that for small amounts of R (near the $R = 0$ point, that is, the singularity) the eigenfunctions will behave simply as

$$\psi_E(R) \sim R^{-\frac{1}{2}}\left(AR^{-i\mu} + BR^{i\mu}\right), \tag{160}$$

where

$$\mu = \frac{1}{2}\left(\frac{48E^2}{\hbar^2} - 1\right)^{1/2} \geq 0. \tag{161}$$

What we mentioned here, indicates that at least on these eigenstates, one cannot set a boundary term of the from $\psi_E(0) = 0$.

Let us have some words about the effect of quantization on the gravitational collapse, which have been exhibited classically by our model. If we are given some state $\psi(R)$, what does it mean to say a measurement leads to the singular (collapsed) geometry? In our procedure, we defined a Hilbert space, hence the quantity $|\psi(R)|^2$ can be interpreted as a probability density. This probability is written as

$$P_\epsilon \equiv \int_0^\epsilon |\psi(R)|^2 \, \mathrm{d}R. \tag{162}$$

The above equation actually gives us the probability that if someone measures R, it will lie in the interval $[0, \epsilon]$. One might wonder if $\psi(0) = 0$ leads to the absence of singularity or not. Well, it does not. To think that it does, is an incorrect interpretation in a case where the spectrum of R is continuous. We can say that when $P_\epsilon \to 0$ then $\epsilon \to 0$. Arguably, the vanishing of ψ at $R = 0$ tends to increase the rate at which P_ϵ tends to zero. We can investigate this kind of behavior for any self-adjoint operator which corresponds to an observable that has a well-defined value at the singularity point. This kind of investigation can be done by putting the spectral theorem into use, and writing the state vector as a function which is located on the spectrum. If the spectrum we are considering happens to have an isolated point (which corresponds to the singular value), then the vanishing of the wave function at that isolated point could indicate the absence of collapse in that state.

So, what does evolution into a singularity mean in quantum theory? We know enough to understand there is uncertainty about it, which makes it difficult for us to say much about the true interpretation of our model for the gravitational collapse. If one finds a wave packet in which some neighborhood of the singularity ($R = 0$) is always avoided by its time evolution (so $P_\epsilon = 0$ for ϵ less than some finite value), then we could claim to have a non-collapsing situation. On the other hand, all of the various wave packets that we have constructed so far, tail down to $R = 0$ in the evolution of time.

Conclusion

There is an important question that one might ask at this point: What did we learn from this article? In this article, we provided some important basic knowledge that is necessary to understand what we should do when we want to try constructing a quantum model for general relativity. Reparametrization invariance, constraints, choice of time, and quantizing the gravitational field were the main subjects. We also faced some problems and obstacles (singularities are an example) while constructing our theories. If one is interested to construct a quantum gravity theory, then it is obvious that overcoming these kinds of obstacles is crucial. It requires lots of hard work and persistence for a physicist to become able to do some valuable work in the act of quantizing the gravitational field. People have been working in this field of science for several decades. What kind of physics are we going to study while living in the next decades ahead of us? Nobody can express a certain answer to this question, however, we can demonstrate some predictions about the future of our scientific frontier.

What is there to achieve? Will our efforts finally cause a paradigm shift in our knowledge in the near future? How can we test our theories and models using experiments? Let us end this article with a quote from Richard Feynman:

> "It doesn't matter how beautiful your theory is, it doesn't matter how smart you are. If it doesn't agree with experiment, it's wrong."

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