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Certificate of Examination

This is to certify that the dissertation titled **[Title of MS Thesis]** submitted by **Aditya Dev** (Reg. No. MS19022) for the partial fulfillment of BS-MS Dual Degree programme of the institute, has been examined by the thesis committee duly appointed by the institute. The committee finds the work done by the candidate satisfactory and recommends that the report be accepted.

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Declaration

The work presented in this dissertation has been carried out by me under the joint supervision of **Dr. Abhishek Chaudhuri** at the Indian Institute of Science Education and Research, Mohali, and **Prof. Dr. Jan Micheal Rost** at Max Planck Institute for the Physics of Complex Systems, Dresden Germany.

This work has not been submitted in part or in full for a degree, a diploma, or a fellowship to any other university or institute. Whenever contributions of others are involved, every effort is made to indicate this clearly, with due acknowledgment of collaborative research and discussions. This thesis is a bonafide record of my original work, and all sources listed within have been detailed in the bibliography.

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In my capacity as the supervisor of the candidate's project work, I certify that the above statements by the candidate are true to the best of my knowledge.

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Abstract

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Chapter 1

Introduction

The unification of Quantum Mechanics and General Relativity has long been the Holy Grail of physics since their development. Despite extensive research, no satisfactory theory has yet been proposed to solve this challenge. General relativity states that a physical theory should not depend on background structures. However, conventional quantization methods often introduce background structures, such as imposing the canonical commutation relations on constant-time hypersurface. The Hamiltonian of a generally covariant theory, such as general relativity, is constrained to vanish in the absence of boundaries [Gielen 23]. Attempts to quantize gravity using canonical quantization lead to a Hamiltonian constraint, the Wheeler-DeWitt equation (i.e., $\mathrm{H}\,|\Psi\rangle\!\rangle = 0$). This leads to an infamous problem known as "The problem of time" in the canonical approach to quantum gravity [Refer to Appendix A for more details]. The issue is that quantum states of space-time (and matter in it) do not seem to undergo any time evolution, as dictated by the constraints of the theory.

In quantum cosmology, the universe is described by a wave function whose dynamics is governed by the Wheeler-DeWitt equation, the quantized Hamiltonian constraint of the system. Due to inherent mathematical ambiguities in the Wheeler-DeWitt equation, it is often unreliable to extend beyond the semi-classical approximation [Cooke 10]. The wave function in this approximation is provided by the WKB wave function, $\Psi_{\mathrm{WKB}} \approx \exp\left[iS_0/\hbar\right]\psi(\{x_n\})$; where S_0 is a function which obeys the classical Hamilton-Jacobi equation for the gravitational field [Gielen 23]. Then we substitute this WKB analysis into the Wheeler-DeWitt equation and applying the relevant approximations leads to the time-dependent Schrödinger equation. Briggs and Rost [Briggs 01] have proposed a similar solution to the problem from an atomic and molecular physics perspective, and their approach is discussed in Chapter 2.

On the other hand, for locally relativistic quantum field theories, it has been demonstrated that the long-range Coulomb field causes the total "charge" opera-

tor to commute with all quasi-local observables, implying a superselection rule for charges [Strocchi 74] [Refer to Appendix B for further details]. Analogously, due to the coupling of energy with the long-range gravitational field, there is speculation about the existence of a superselection rule for energy [Page 83]. This implies that only operators that commute with the Hamiltonian can be observable. However, such observables are stationary (i.e., constants of motion). How can we observe time evolution if the only observables we can observe are stationary i.e., they do not evolve at all?

The problem of time is a manifestation of background independence rather than the "timelessness" of quantum mechanics, and means that physical states do not evolve relative to an external background time. Instead, time evolution must be extracted relationally, by selecting certain quantized degrees of freedom to serve as an internal timekeeper, i.e., pick some quantized degrees of freedom to serve as an internal time. Even in our everyday "classical' world, we never directly measure time; instead, we measure the position or angular displacement of a pendulum or a dial and use that measurement to *define* a unit of time. The use of relational time in Quantum Mechanics is a framework in which one promotes all variables to quantum operators and later chooses one of the variables to operate like a "clock" degree of freedom.

Apart from the semi-classical approaches employed in quantum cosmology, various other avenues exist to address the time problem from a purely quantum mechanical standpoint [Höhn 21]. One such approach is the "Page-Wootters Formalism" (abbreviated P&W formalism), which defines relational dynamics in terms of conditional probabilities for the clock and evolving degrees of freedom [Page 83]. To date, no one has successfully tackled the problem involving general interaction potentials [with the exception of [Smith 19] to a certain extent]. The original formulation due to P&W is no exception, as it also neglects the interaction between the environment and the system. However, recent work by Gemsheim and Rost has developed a relational formalism based on the P&W formalism, which now includes the environment-system interaction [Gemsheim 23]. This advancement provides the necessary tools to study relational dynamics for a general system-environment setting. Their approach is discussed in detail in Chapter 3.

The primary objective of this work is to study the transition from quantum mechanical approach to semi-classics, in the limit of a large environment[1]

[1]The notion of a "large" environment will be elaborated upon in subsequent chapters.

Chapter 2

Emergence of Time dependence through interaction with a Semi-classical Environment

In modern textbooks, the Time-dependent Schrödinger equation (TDSE) is either introduced as a *fundamental* equation governing the time evolution of a quantum wave function, with the Time-independent Schrödinger equation (TISE) as a special case, or it is derived from the correspondence with classical Hamilton-Jacobi theory.

Briggs and Rost [Briggs 01] presented an alternative derivation of the TDSE that partitions the "global" Hilbert space into a system and an environment. They then employed the WKB ansatz for the environment's wave function, effectively treating the environment semi-classically. Their analysis offers a clear physical interpretation of the time parameter, which arises from a directional gradient of the classical action along the environment trajectory. This chapter presents the analysis by Briggs and Rost in [Briggs 01].

Consider a global system with Hamiltonian H, which comprises a system S and an environment $\mathcal{E}$. The TISE for this system is given by

$$\mathrm{H}\,\Psi = E\Psi, \quad \mathrm{H} = \mathrm{H}_S + \mathrm{H}_{\mathcal{E}} + \mathrm{H}_{\mathcal{SE}}\,. \tag{2.1}$$

where H_S and $\mathrm{H}_{\mathcal{E}}$ are the Hamiltonians of the system and the environment respectively and $\mathrm{H}_{\mathcal{SE}}$ is the interaction Hamiltonian between the system and the environment[1].

The total wave function Ψ can be written as

$$\Psi(x, R) = \sum \psi_m(x, R)\chi_m(R). \tag{2.2}$$

[1] $\mathrm{H}_{\mathcal{SE}} \equiv \mathrm{H}_{\mathcal{SE}}(x, R)$

Where $\{\psi's\}$ represent the energy eigenstates of $\mathrm{H}_{\mathcal{S}}+\mathrm{H}_{\mathcal{SE}}$ at a fixed R, with $\epsilon_n(R) = \langle\psi_n|\,\mathrm{H}_{\mathcal{S}}+\mathrm{H}_{\mathcal{SE}}\,|\psi_n\rangle$, and x and R represent the coordinates of the system and the environment, respectively. [2]. The environment Hamiltonian is assumed to be of the form

$$\mathrm{H}_{\mathcal{E}} = \mathrm{K}+\mathrm{V}_{\mathcal{E}}(R). \tag{2.3}$$

with:

$$\mathrm{K} = \frac{-\hbar^2}{2M}\sum_i \frac{\partial^2}{\partial R_i^2} = \frac{-\hbar^2}{2M}\nabla_R^2. \tag{2.4}$$

Substituting Eqn. 2.2 in Eqn. 2.1 and projecting onto $\psi_n(x,R)$ gives a coupled TISE for the environment wavefunction[3] [Briggs 01]:

$$\begin{aligned}\sum_m \langle\psi_n|\left(\frac{-\hbar^2}{2M}\nabla_R^2\right)|\psi_m\rangle\,\chi_m(R) + \mathrm{V}_{\mathcal{E}}(R)\chi_n(R)\\ +\sum_m \langle\psi_n|\,\mathrm{H}_{\mathcal{S}}+\mathrm{H}_{\mathcal{SE}}\,|\psi_m\rangle\,\chi_m(R) = E\chi_n(R).\end{aligned} \tag{2.5}$$

The "potentials":

$$\mathcal{V}_{mn}(R) = \langle\psi_m|\,\mathrm{H}_{\mathcal{S}}+\mathrm{H}_{\mathcal{SE}}\,|\psi_n\rangle\,. \tag{2.6}$$

depending on the state of the quantum system, provide the energy surface which determines the dynamics of the environment. The coupling from the kinetic term is

$$\begin{aligned}&\langle\psi_m|\left(\frac{-\hbar^2}{2M}\nabla_R^2\right)|\psi_n\rangle\,\chi_n(R)\\ &= -\frac{\hbar^2}{2M}\sum_k \left(\delta_{mk}\nabla_R + \langle\psi_m|\,\nabla_R\,|\psi_k\rangle\right)\left(\delta_{kn}\nabla_R + \langle\psi_k|\,\nabla_R^2\,|\psi_n\rangle\right)\chi_n(R).\end{aligned} \tag{2.7}$$

We define

$$\Lambda_{mn}(R) = i\hbar\,\langle\psi_m|\,\nabla_R\,|\psi_n\rangle\,. \tag{2.8}$$

Now, using above definitions, Eqn. 2.5 can be written as

$$\sum_m\left[\frac{1}{2M}(\hat{P}^2)_{nm} + \mathcal{V}_{nm}(R)\right]\chi_m(R) + \mathrm{V}_{\mathcal{E}}(R)\chi_n(R) = E\chi_n(R). \tag{2.9}$$

Where

$$\hat{P}_{nm} = -i\hbar\left(\mathbb{I}\nabla_R - \frac{i}{\hbar}\hat{\Lambda}\right) = \left(\mathbb{I}P_R - \hat{\Lambda}\right) \quad \text{or} \quad P_{ij} = \left(\delta_{ij}P_R - \Lambda_{ij}\right). \tag{2.10}$$

Notice that the kinematic coupling $\hat{\Lambda}$ appears as a vector potential.

[2] We have assumed that the environment is large enough so the system has a no effect on the environment's states. Furthermore, $\langle\chi_m|\chi_n\rangle \neq \delta_{mn}$.

[3] Notice that, we integrate only over x.

The set of equations for system wavefunction is given by

$$\sum_m \chi_m(R)\left[\mathrm{H}_{\mathcal{S}}+\mathrm{H}_{\mathcal{SE}}(x,R)-\left(E-\mathrm{V}_{\mathcal{E}}(R)+\frac{1}{\chi_m}\frac{\hbar^2}{2M}\nabla_R^2\chi_m\right)\right.$$
$$\left.-\frac{\hbar^2}{2M}\nabla_R^2-\frac{\hbar^2}{M\chi_m}\nabla_R\chi_m\cdot\nabla_R\right]\psi_m(x,R)=0. \quad (2.11)$$

The main approximation in this derivation would be to disentangle Eqn. 2.9 and Eqn. 2.11. To do so, we assume that the environment is large enough so that the changes in the system, i.e. the variation in matrix elements $\mathcal{V}_{mn}$ and Λ_{mn}, have no effect on the environment dynamics.

The fist step would be to neglect in Eqn. 2.9 all the off-diagonal matrix elements, which gives:

$$\left[\frac{1}{2M}\left(P_R-\Lambda_{nn}(R)\right)^2+\mathrm{V}_{\mathcal{E}}+E_n(R)\right]\chi_n(R)=E\chi_n(R). \quad (2.12)$$

with $E_n(R)=\mathcal{V}_{nn}(R)$. The vector potential Λ_{nn}, since now diagonal in the above case, can be included in the definition of an effective environment momentum operator.

The second step would be to use a semi-classical approximation for each $\chi_m(R)$, i.e., we write

$$\chi_n(R)=a_n(R)\exp\left(\frac{i}{\hbar}W_n(R)\right)\equiv\exp\left(\frac{i}{\hbar}W(R,E-\epsilon_n)\right). \quad (2.13)$$

with

$$\nabla_R W_n=\boldsymbol{P}_n. \quad (2.14)$$

where the classical momentum $\boldsymbol{P}_n$ and position $\boldsymbol{R}_n$ are decided by Hamilton's equations:

$$\frac{d\boldsymbol{P}_n}{dt} = -\nabla_{R_n}H=\nabla_{R_n}\left(\mathrm{V}_{\mathcal{E}}(R)+E_n(R)\right) \quad (2.15)$$
$$\frac{d\boldsymbol{R}_n}{dt} = \nabla_{P_n}H. \quad (2.16)$$

For the standard kinetic energy $\frac{\boldsymbol{P}^2}{2M}$, one obtains from Eqn. 2.16 that $\boldsymbol{P}_n=M\frac{d\boldsymbol{R}_n}{dt}$. It is at this point that the time parameter enters the picture. To the leading order in $\hbar$, one can write:

$$\frac{\hbar}{iM}\nabla_R\chi_n=\frac{\chi_n}{a_n}\frac{\hbar}{iM}\nabla_R a_n+\chi_n\frac{1}{M}\nabla_R W_n\approx\chi_n\frac{d\boldsymbol{R}_n}{dt}. \quad (2.17)$$

For the system $\mathcal{S}$ the equation coupled to Eqn. 2.12 now reads

$$\sum_m\chi_m(R)\left[\mathrm{H}_{\mathcal{S}}+\mathrm{H}_{\mathcal{SE}}(x,R)-E_m(R)-\frac{\hbar^2}{2M}\nabla_R^2-i\hbar\frac{d\boldsymbol{R}_m}{dt}\cdot\nabla_R\right]\psi_m(x,R)=0. \quad (2.18)$$

It has been shown [Briggs 01] that in the above equation, the term $(\hbar^2/2M)\nabla_R^2$ with higher-order gradient couplings can be neglected in comparison with the term

$$i\hbar\frac{d\boldsymbol{R}_n}{dt}\cdot\nabla_R := i\hbar\frac{d}{d\tau_n}.$$

Hence, Eqn. 2.18 can be written as

$$\sum_m \chi_m(R)\left[\mathrm{H}_{\mathcal{S}}+\mathrm{H}_{\mathcal{SE}}(x,\{\tau_m\})-E_m(\{\tau_m\})-i\hbar\frac{\partial}{\partial\tau_m}\right]\psi_m(x,R)=0. \tag{2.19}$$

We have replaced the quantum R dependence by a “classical time" like dependence on $\{\tau_m\}$.

In the approximation represented by Eqn. 2.14 and Eqn. 2.19, the environment shows classical dynamics, but the state of the quantum system determines its motion and, hence, the interaction time with the system. This represents the final impact of the quantum influence on the environment. This influence diminishes as the environment becomes fully disentangled from the system, allowing it to function as an external clock that reads a unique time [Briggs 01].

This simplification is achieved in the approximation when Eqn. 2.13 becomes

$$\chi_n(R)=a_n(R)\exp\left(\frac{i}{\hbar}W(R)\right). \tag{2.20}$$

which is valid in the limit $\epsilon_n \ll E$. It is at this point that the Environment gets fully disentangled from the system. Then we get from Eqn. 2.20, a unique time derivative

$$\nabla_R W = M\frac{d\boldsymbol{R}}{dt} \tag{2.21}$$

Also, one can eliminate $E_m(t)$ using a purely time-dependent phase transformation and writing $\psi_{\mathcal{S}}(x)=\sum_n a_n\psi_n(x)$, Eqn. 2.19 becomes:

$$\left[\mathrm{H}_{\mathcal{S}}+\mathrm{H}_{\mathcal{SE}}(x,t)-i\hbar\frac{\partial}{\partial t}\right]\psi_m(x,t)=0 \tag{2.22}$$

This gives the TDSE for the quantum system alone. Now, the dynamics of the environment is given by the classical equation of motion, with the system having no effect on it. However, the quantum system is affected by the environment through the term $\mathrm{H}_{\mathcal{SE}}$

Chapter 3

Relational Quantum Mechanics: With System and Environment Interaction

[*Please note that the words 'clock' and 'environment' will be used synonymously. The term "system" denotes a subsystem (excluding the environment) of a global Hilbert space unless otherwise specified.*]

We start by *reformulating* the time independent Schrödinger equation as an *invariance principle* [Gemsheim 23]

$$\exp\left[i\lambda(\mathrm{H} - E\mathrm{I})\right]|\Psi\rangle\!\rangle = |\Psi\rangle\!\rangle\,. \tag{3.1}$$

Where λ is any complex-valued parameter, H is the Hamiltonian of the global system, and $|\Psi\rangle\!\rangle$ is the global state vector. Differentiating (Eqn. 3.1) with respect to λ one gets the usual Time Independent Schrödinger Equation (TISE)

$$\mathrm{H}\,|\Psi\rangle\!\rangle = E\,|\Psi\rangle\!\rangle\,.$$

For our analysis, we assume that is real. We partition the total Hilbert space $\mathcal{H}$ into two components to extract the dynamics. A system $\mathcal{H}_s$ and a clock $\mathcal{H}_c$. We re-write

$$\mathrm{H} = \mathrm{H}_s \otimes \mathrm{I}_c + \mathrm{I}_s \otimes \mathrm{H}_c + \mathrm{V}. \tag{3.2}$$

Since the system and environment are embedded in the global Hilbert space, one can single out the system state by projecting the global state partially onto a static state of the environment.

For non-interacting system and environment: Let $|\chi\rangle$ be a state vector in clock Hilbert space.

We choose some state $|\chi_0\rangle \in \mathcal{H}_c$. If one projects the state vector $|\chi_0\rangle$ onto the invariance equation (Eqn. 3.1) (assuming the absence of interaction, represented by

$\mathrm{V} = 0$), one gets

$$\begin{aligned} \langle\chi_0|\, e^{i\lambda(\mathrm{H}-E)}\, |\Psi\rangle\!\rangle &= \langle\chi_0|\Psi\rangle\!\rangle \\ \langle\chi_0|\, e^{i\lambda(\mathrm{H}_c-E)}\, |\Psi\rangle\!\rangle &= e^{-i\lambda \mathrm{H}_s}\, \langle\chi_0|\Psi\rangle\!\rangle\,. \end{aligned} \tag{3.3}$$

We define

$$|\chi_\lambda\rangle = e^{-i\lambda(\mathrm{H}_c-E)}\, |\chi_0\rangle\,. \tag{3.4}$$

By conditioning the global state $|\Psi\rangle\!\rangle$ onto a clock state $|\chi_\lambda\rangle$, we utilize the state $|\chi_\lambda\rangle$ as a label to associate the system state with the particular value of λ, i.e.,

$$|\varphi(\lambda)\rangle_s \equiv \langle\chi_\lambda|\Psi\rangle\!\rangle\,. \tag{3.5}$$

So,

$$|\varphi(\lambda)\rangle_s = e^{-i\lambda \mathrm{H}_s}\, \langle\chi_0|\Psi\rangle\!\rangle \equiv e^{-i\lambda \mathrm{H}_s}\, |\varphi(0)\rangle_s\,. \tag{3.6}$$

Notice that the choice of $|\chi_0\rangle$ fixes the system's initial state. Since, λ in (Eqn. 3.6) is assumed to be a continuous parameter, the above equation can be interpreted as a solution to the differential equation

$$i\frac{d}{d\lambda}\, |\varphi(\lambda)\rangle_s = \mathrm{H}_s\, |\varphi(\lambda)\rangle_s\,. \tag{3.7}$$

Which is equivalent to (Time-dependent Schrödinger Equation) TDSE in units $\hbar = 1$. It is crucial for the system and the environment within the global Hilbert space to exhibit entanglement. Otherwise, the system and the environment would uphold separate "global" invariance principles, each with its own parameter, λ_s and λ_c, respectively. This would leave the relationship between λ_s and λ_c unresolved [Gemsheim 23].

Role of parameter λ: The variable λ introduced in the above derivation has no physical significance. It only serves as a parameter to track the evolution of our system. Any reparametrization of $\lambda \to t(\lambda)$ has no change in the equation of the system state evolution. One can, in principle [1] parameterize the evolution using an observable of our environment $\mathrm{A}_c(\lambda) \equiv \langle\chi_\lambda|\, \mathrm{A}_c\, |\chi_\lambda\rangle$. An ideal choice would be to use such a A_c for which the relation between λ and A_c is simple, for example, linear.

High-resolution clock states $|\chi_\lambda\rangle \propto \sum_k a_k \exp(-i\lambda E_c^k)\, |E_c\rangle_k$ require a broad distribution over the clock energy eigenstates, ideally with uniform coefficients (a_k) [Gemsheim 23, Smith 19]. This condition is readily met when the clock's physical dimensions exceed those of the system.

[1] As one does it always. We never measure time directly; rather, we measure the angular position of a clock dial or the no of transition electrons made in a cesium atom.

For interacting system and environment: So far in our analysis, we have assumed no interaction, i.e., $\mathrm{V} = 0$. However, in real scenarios, one always has some interaction within components of a global closed system. To extend the derivation to non-zero V, we modify our clock state as

$$\begin{aligned} |\chi_\lambda\rangle = e^{-i\lambda(\mathrm{H}_c - E)} |\chi_0\rangle \rightarrow \\ |\chi_\lambda\rangle = e^{-iS(\lambda)} e^{-i\lambda(\mathrm{H}_c - E)} |\chi_0\rangle \end{aligned} \tag{3.8}$$

where $S(\lambda) = \int^\lambda \xi(\tilde{\lambda}) d\tilde{\lambda}$ is an extra factor introduced for simplifying upcoming derivations. When projected onto this, the global state can be written as

$$\left(-\mathrm{H}_s + \xi(\lambda) + i\frac{d}{d\lambda}\right) \langle\chi_\lambda|\Psi\rangle\!\rangle = \langle\chi_\lambda| \mathrm{V} |\Psi\rangle\!\rangle \,. \tag{3.9}$$

We can rearrange the above equation to write it as

$$i\frac{d}{d\lambda} \langle\chi_\lambda|\Psi\rangle\!\rangle = \mathrm{H}_s \langle\chi_\lambda|\Psi\rangle\!\rangle - \xi(\lambda) \langle\chi_\lambda|\Psi\rangle\!\rangle + \langle\chi_\lambda| \mathrm{V} |\Psi\rangle\!\rangle \,. \tag{3.10}$$

We now decompose $\langle\chi_\lambda| \mathrm{V} |\Psi\rangle\!\rangle$ into a Hermitian potential and a c-number. To facilitate the decomposition, we define the following:

$$\begin{aligned} \mathrm{P}_\Psi = |\Psi\rangle\!\rangle \langle\!\langle\Psi| \,, \quad \mathrm{P}_\chi = \mathrm{I}_s \otimes |\chi_\lambda\rangle \langle\chi_\lambda| \\ \mathrm{P}_{\Psi\chi} = \mathrm{P}_\Psi \mathrm{P}_\chi / \mathcal{N}_\lambda \end{aligned} \tag{3.11}$$

where $\mathcal{N}_\lambda = \langle\!\langle\Psi| \mathrm{P}_\chi |\Psi\rangle\!\rangle$. One observes that

$$\mathrm{P}_{\Psi\chi} |\Psi\rangle\!\rangle = \frac{\mathrm{P}_\Psi \mathrm{P}_\chi}{\mathcal{N}_\lambda} |\Psi\rangle\!\rangle = |\Psi\rangle\!\rangle \tag{3.12}$$

Using above defined operators, we decompose the

$$\begin{aligned} \langle\chi_\lambda| \mathrm{V} |\Psi\rangle\!\rangle = \langle\chi_\lambda| \mathrm{V}\mathrm{P}_{\Psi\chi} |\Psi\rangle\!\rangle \\ = \left[\mathrm{V}_s(\lambda) - \langle\!\langle\Psi| \mathrm{V}\mathrm{P}_\chi |\Psi\rangle\!\rangle / \mathcal{N}_\lambda\right] \langle\chi_\lambda|\Psi\rangle\!\rangle \end{aligned} \tag{3.13}$$

where

$$\mathrm{V}_s(\lambda) = \frac{\langle\chi_\lambda| \left(\mathrm{V}\mathrm{P}_\Psi + \mathrm{P}_\Psi \mathrm{V}\right) |\chi_\lambda\rangle}{\mathcal{N}_\lambda}$$

Inserting (Eqn. 3.13) into (Eqn. 3.10) and setting $\xi(\lambda) = -\langle\!\langle\Psi| \mathrm{V}\mathrm{P}_\chi |\Psi\rangle\!\rangle / \mathcal{N}_\lambda$ we obtain

$$\boxed{i\frac{d}{d\lambda} |\varphi(\lambda)\rangle_s = \left[\mathrm{H}_s + \mathrm{V}_s(\lambda)\right] |\varphi(\lambda)\rangle_s}, \tag{3.14}$$

where we defined $\langle\chi_\lambda|\Psi\rangle\!\rangle = |\varphi(\lambda)\rangle_s$. The phase factor $S(\lambda) = \int^\lambda \xi(\tau) d\tau$ introduced helps eliminate the c-number after the decomposition of the "effective" potential.

We find that the final form of the Equation is equivalent to the TDSE for the remaining sub-system ($\mathcal{H}_s$) of the global Hilbert space $\mathcal{H}$.

Chapter 4

Open Questions, Progress Made and Future Prospects

The primary objective of this work is to investigate the transition from purely quantum systems, as explored in Chapter 3, to semi-classical regimes, as discussed in Chapter 2 and, to compare the dynamics as described by the two approaches. However, a crucial question arises: What type of clocks (i.e., “Environments”) are we considering in this context? Also, one notices that, as shown in Chapter 3, the “emergent" potential in Eqn 3.14 depends on the clock state on which the global system is projected. So, a natural question would be to ask: What type of clock states would one use? Especially in the context of our work?

The phase of the WKB wave function, which satisfies the Hamilton-Jacobi equation, implies that the argument (x) corresponds precisely to the classical trajectory of the clock system. Consequently, a natural approach would be to employ environment Hamiltonian for which we can define specific “special” states such that the expectation values of observables coincide with the classical trajectories. For instance, the coherent states of harmonic oscillators are suitable candidates [Braun 04]. Furthermore, these states are preferable due to their well-defined position representation *although the necessity of this requirement remains an open question*.

Given the wide range of potential environments, two generic environment systems are discussed in the following sections.

4.1 Spin Systems

In the context of semi-classical clocks, we can either take a single “large spin" with angular momentum (l) or a spin chain composed of (N) small spins.

For the former, taking the limit $l \to \infty \Rightarrow d_C \to \infty$ allows us to consider the clock

Hilbert space to become infinite-dimensional, making it a suitable candidate for a large environment. Similarly, for the latter, taking the limit $N \to \infty \Rightarrow d_C \to \infty$ leads to the same result.

However, careful consideration must be given to the representation in which the clocks are described. As the WKB approximation always assumes, the WKB wave function is in position representation. So, we have a specific choice of representation. This can be challenging for spin systems, as quantum spins are intrinsic properties of quantum particles and lack a direct classical counterpart.

Unlike angular momentum operators, which inherit their position representation from the position representation of x and p, it is not possible to express S_z in terms of the classical position and momenta. This is because spin is an intrinsic rather than a spatial degree of freedom. Dimensional analysis shows that only products like yp_x have units of angular momentum so, after incorporating the commutation relations, a position representation of spin would closely resemble the position representation of "ordinary" angular momentum, with spherical harmonics serving as the eigenstates for the angular momentum operator. However, caution is advised, as spherical harmonics are only defined for integer values of angular momentum, rendering the representation invalid for half-integer values of angular momentum.

Another promising approach, I will investigate, is the method of WKB for spin in terms of a spectral representation [Van Hemmen 86, Van Hemmen 03] which offers a means of defining the WKB wave function in the large spin limit as discussed above. Details of this approach are still being worked on.

4.2 Quantum Harmonic Oscillator

Another candidate for the environment would be to use truncated quantum harmonic oscillators (QHOs) as clocks. Similarly to spin systems, one could use a single "large Quantum Harmonic Oscillator" or a chain of "small quantum harmonic oscillators".4for

An immediate advantage of using a Quantum Harmonic Oscillator is that the position representation is well-defined. As discussed at the beginning of the chapter, the coherent states are the best candidates for the clock states to which the global states will be projected. This is because the expectation values of the coherent states' position and momentum operators are exactly the clock system's classical trajectories. Rovelli [Rovelli 90] and Ashworth [Ashworth 98] have explored a comparable perspective on the concept of a clock, although within the framework of non-interacting systems.

4.3 Progress made and Future Work

The following list summarizes the future work that needs to be done:

Numerical Implementation Numerical implementation of the relational approach for general finite-dimensional systems has been implemented in the `Python` and `Julia` programming language. Some code checks have been performed to ensure the correctness of the implementation.

Future work in this direction includes:

- Extend the numerical implementation of the relational approach for finite dimensional systems to include the case of large spin systems.
- Investigate the limitations on the size of the systems that can be simulated numerically.

Analytical Work

- The analytical work for the systems as mentioned above is still in progress. The WKB method for the case of a spin system is still being worked on. The approach of [Van Hemmen 86] provides an interesting way of writing the WKB wave function for the large spin limit. The details of this approach need to be worked out, for how to include it in our relational formalism from both numerical and analytical perspectives.
- One also needs to formulate analytical or numerical work on how the comparison between the two approaches can be done in a more quantitative way.

Appendix A

The Problem of Time

Action principles are widely used to express the laws of physics, including those of general relativity. Symmetry transformations are changes in the coordinates or variables that leave the action invariant. It is well known that continuous symmetries generate conservation laws (Noethers Theorem). Conservation laws are of fundamental importance in physics, and so it is valuable to investigate the symmetries of the action.

It is useful to distinguish between two types of symmetries: *dynamical symmetries* corresponding to some inherent property of matter or spacetime evolution (e.g., the Lagrangian being independent of a coordinate, leading to a conserved conjugate momentum) and *non-dynamical symmetries* arising because of the way in which we formulate the action (e.g., the gauge symmetries). Dynamical symmetries constrain the solutions of the equations of motion, while non-dynamical symmetries give rise to special laws called identities. They are distinct from conservation laws because they hold regardless of whether or not one has extremized the action.

Parameterization-Invariance and Hamiltonian Constrain

Consider a system with n degrees of freedom - the generalized coordinates q_i - with a parameter t giving the evolution of the trajectory in configuration space. We will remove the superscript on q_i when it is clear from the context. Let the action of this system be:

$$\mathcal{S} = \int L_s \left(q, \frac{dq}{dt} \right) dt \tag{A.1}$$

Now consider a new integration parameter τ, which now parameterize the trajectory and promote $t \to t(\tau)$ i.e to a dynamical variable. In terms of τ the action (Eqn. A.1)

can be expressed as:

$$\mathcal{S} = \int L_s\left(q, \frac{\dot{q}}{\dot{t}}\right) \dot{t} d\tau = \int L\left(q, \dot{q}, \dot{t}\right) d\tau \tag{A.2}$$

where $\dot{a} \equiv \dfrac{da}{d\tau}$ and $L\left(q, \dot{q}, \dot{t}\right) = \dot{t} L_s\left(q, \frac{\dot{q}}{\dot{t}}\right)$. The Hamiltonian for the modified Lagrangian is then obtained by taking the Legendre transformation w.r.t. both $\dot{q}$ and $\dot{t}$ [Deriglazov 11]:

$$\begin{aligned} H &= p_t \dot{t} + p_q \dot{q} - L \\ H &= p_t \dot{t} + \dot{t} p_q (\dot{q}/\dot{t}) - \dot{t} L_s \\ H &= \dot{t}\left(p_t + p_q q' - L_s\right) \end{aligned} \tag{A.3}$$

where $q' = \dfrac{dq}{dt} = (\dot{q}/\dot{t})$.

Let's calculate the conjugate momenta:

$$\begin{aligned} p_q := \frac{\partial L}{\partial \dot{q}} = \dot{t}\frac{\partial L_s}{\partial \dot{q}} &= \frac{\partial L_s}{\partial (\dot{q}/\dot{t})} \\ p_q &= \frac{\partial L_s}{\partial q'} \end{aligned} \tag{A.4}$$

which coincides with the momentum conjugate to q defined by $L_s(q, q')$. Hence, (Eqn. A.3) get's modified as:

$$H = \dot{t}\left(p_t + H_s\right) \tag{A.5}$$

where $H_s = p_q q' - L_s$ i.e Hamiltonian conjugate to L_s.

We have:

$$\begin{aligned} p_t &:= \frac{\partial L}{\partial \dot{t}} \\ p_t &= L_s + \dot{t}\frac{\partial L_s(q, q')}{\partial \dot{t}} \\ p_t &= L_s + \dot{t}\left(\frac{\partial L_s(q, q')}{\partial q}\overbrace{\frac{dq}{d\dot{t}}}^{0} + \frac{\partial L_s(q, q')}{\partial q'}\frac{d(\dot{q}/\dot{t})}{d\dot{t}}\right) \\ p_t &= L_s - q' p_s = -H_s \end{aligned} \tag{A.6}$$

Using (Eqn. A.6) in (Eqn. A.5), the equation reduces to:

$$\boxed{H = 0} \tag{A.7}$$

Therefore, for parameterization-invariant theory, the Hamiltonian function is identically zero. It is crucial to note that this *derivation makes no assumptions about the extremality of the action or the satisfaction of the Euler-Lagrange equations* by the (q's). Consequently, Eqn. A.7 represents a non-dynamical symmetry.

Identity $H = 0$ is very different from conservation law $H = \text{constant}$ arising from a time-independent Lagrangian. The conservation law holds only for solutions of

the equations of motion; in contrast, when the action is parameterization-invariant, $H = 0$ holds for any trajectory. The non-dynamical symmetry, therefore, does not constrain the motion.

Appendix B

Super-Selection Rule

In quantum theory, physically measurable quantities of a microscopic system are represented by self-adjoint operators. However, not all of the self-adjoint operators correspond to measurable quantities. The super-selection rule is a criterion to distinguish measurable self-adjoint operator from the un-measurable ones, i.e., any measurable quantity must obey the superselection rules. By contraposition, any quantity which does not obey the superselection rules cannot be measured. It should be noted that such a statement implies that the set of (physically realizable) observables is strictly smaller than the set of all self-adjoint operators on Hilbert space. The notion of superselection rule (henceforth abbreviated SSR) was first introduced in 1952 by Wick, Wightman, and Wigner [Wick 52] in connection with the problem of consistently assigning intrinsic parity to elementary particles.

In the context of quantum field theory, the electric current $J^\mu = \overline{\psi}\gamma^\mu\psi$ is defined in terms of the Dirac spinor field operator ψ for electrons. The electric current J^μ is self-adjoint and measurable. However, the operators

$$\frac{1}{2}\left(\psi + \psi^\dagger\right) \qquad \frac{1}{2i}\left(\psi - \psi^\dagger\right) \tag{B.1}$$

are also self-adjoint but they are not measurable even via indirect methods.

A SSR is stated as follows: There is an operator J, which we call the superselection charge. If a self-adjoint operator A represents a measurable quantity, it must satisfy the commutativity [Tanimura 11]

$$[\mathrm{J}, \mathrm{A}] = 0 \tag{B.2}$$

This is a SSR, which is a necessary condition for the measurability of A. The SSR can be compared with a conservation law. The conservation of J is formulated as

$$[\mathrm{J}, \mathrm{H}] = 0 \tag{B.3}$$

where H is the Hamiltonian H of the system. The conservation law (Eqn. B.3) requires that J commutes with the Hamiltonian H while the superselection rule (Eqn. B.2) requires that J commutes with all of the measurable quantities. Thus, the superselection rule is a stronger requirement for J than the conservation law. It can be said that the superselection rule is an extreme form of conservation laws.

Notice that the SSR (Eq Eqn. B.2) implies that, for all physically measurable observables A and any eigenvector $|\psi_i\rangle$ of J with charge q_i[1].

$$\begin{aligned} \langle\psi_i|\,\mathrm{JA}\,|\psi_j\rangle - \langle\psi_i|\,\mathrm{AJ}\,|\psi_j\rangle &= 0 \\ (q_i - q_j)\,\langle\psi_i|\,\mathrm{A}\,|\psi_j\rangle &= 0 \\ \langle\psi_i|\,\mathrm{A}\,|\psi_j\rangle &= 0 \quad (\text{for } i \neq j) \end{aligned} \tag{B.4}$$

So, if we have a quantum state in a coherent superposition of eigenstates of superselection charge J i.e. $|\psi_+\rangle = \frac{|\psi_1\rangle + |\psi_2\rangle}{\sqrt{2}}$. One can check that:

$$\begin{aligned} \langle\psi_+|\,\mathrm{A}\,|\psi_+\rangle &= \frac{\langle\psi_1|\,\mathrm{A}\,|\psi_1\rangle + \langle\psi_2|\,\mathrm{A}\,|\psi_2\rangle + \overbrace{2\mathrm{Re}[\langle\psi_1|\,\mathrm{A}\,|\psi_2\rangle]}^{=0}}{2} \\ \langle\psi_+|\,\mathrm{A}\,|\psi_+\rangle &= \frac{\langle\psi_1|\,\mathrm{A}\,|\psi_1\rangle + \langle\psi_2|\,\mathrm{A}\,|\psi_2\rangle}{2} = \mathrm{Tr}\{\rho\mathrm{A}\} \end{aligned} \tag{B.5}$$

where

$$\rho = \frac{|\psi_1\rangle\langle\psi_1| + |\psi_2\rangle\langle\psi_2|}{2} \tag{B.6}$$

i.e. any relative phase between $|\psi_1\rangle$ and $|\psi_2\rangle$ is not measurable and that coherent superposition of $|\psi_1\rangle$ and $|\psi_2\rangle$ cannot be verified (or prepared). For an observer, the state $|\psi_+\rangle$ will not be any different from a mixed state ρ.

[1] we assume J is non degenerate

Bibliography

[Ashworth 98] M. C. Ashworth. *Coherent state approach to quantum clocks*. Phys. Rev. D, vol. 58, page 104008, 1998. [Cited on page 11]

[Braun 04] Lars Braun, Walter T. Strunz & John S. Briggs. *Classical limit of the interaction of a quantum system with the electromagnetic field*. Phys. Rev. A, vol. 70, page 033814, Sep 2004. [Cited on page 10]

[Briggs 01] John S Briggs & Jan M Rost. *On the derivation of the time-dependent equation of Schrödinger*. Foundations of Physics, vol. 31, pages 693–712, 2001. [Cited on pages 1, 3, 4, and 6]

[Cooke 10] Michael Cooke. An introduction to quantum cosmology. Master's thesis, Imperial College London, 2010. [Cited on page 1]

[Deriglazov 11] A Deriglazov & BF Rizzuti. *Reparametrization-invariant formulation of classical mechanics and the Schrödinger equation*. American Journal of Physics, vol. 79, no. 8, pages 882–885, 2011. [Cited on page 14]

[Gemsheim 23] Sebastian Gemsheim & Jan M. Rost. *Emergence of Time from Quantum Interaction with the Environment*. Phys. Rev. Lett., vol. 131, no. 14, page 140202, 2023. [Cited on pages 2, 7, and 8]

[Gielen 23] Steffen Gielen. *Quantum Cosmology*. arXiv preprint arXiv:2309.01790, 2023. [Cited on page 1]

[Höhn 21] Philipp A Höhn, Alexander RH Smith & Maximilian PE Lock. *Trinity of relational quantum dynamics*. Physical Review D, vol. 104, no. 6, page 066001, 2021. [Cited on page 2]

[Page 83] Don N Page & William K Wootters. *Evolution without evolution: Dynamics described by stationary observables*. Physical Review D, vol. 27, no. 12, page 2885, 1983. [Cited on page 2]

[Rovelli 90] Carlo Rovelli. *Quantum mechanics without time: a model*. Physical Review D, vol. 42, no. 8, page 2638, 1990. [Cited on page 11]

[Smith 19] Alexander R. H. Smith & Mehdi Ahmadi. *Quantizing time: Interacting clocks and systems*. Quantum, vol. 3, page 160, 2019. [Cited on pages 2 and 8]

[Strocchi 74] F. Strocchi & A. S. Wightman. *Proof of the Charge Superselection Rule in Local Relativistic Quantum Field Theory.* J. Math. Phys., vol. 15, pages 2198–2224, 1974. [Erratum: J.Math.Phys. 17, 1930–1931 (1976)]. [Cited on page 2]

[Tanimura 11] Shogo Tanimura. *Superselection rules from measurement theory*. arXiv preprint arXiv:1112.5701, 2011. [Cited on page 16]

[Van Hemmen 86] JL Van Hemmen & A Sütö. *Tunneling of quantum spins*. Physica B+ C, vol. 141, no. 1, pages 37–75, 1986. [Cited on pages 11 and 12]

[Van Hemmen 03] JL Van Hemmen & A Sütö. *WKB for quantum spins*. Physica A: Statistical Mechanics and its Applications, vol. 321, no. 3-4, pages 493–497, 2003. [Cited on page 11]

[Wick 52] G. C. Wick, A. S. Wightman & E. P. Wigner. *The intrinsic parity of elementary particles*. Phys. Rev., vol. 88, pages 101–105, 1952. [Cited on page 16]