Relational Dynamics From Entangled Eigenstates

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Certificate of Examination

This is to certify that the dissertation titled **Relational Dynamics From Entangled Eigenstates** 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, **Prof. Dr. Jan Micheal Rost** and **Dr. Matthew Travis Eiles** 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

Use this section to include an abstract of the thesis. $\phi, \Phi, \varphi, \sigma$

Notations and Conventions

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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., $\mathbf{H}\left|\Psi\right\rangle\!\rangle = 0$). 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 semiclassical 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 ansatz into the Wheeler-DeWitt

equation and applying the relevant approximations leads to the time-dependent Schrödinger equation. The work of Briggs et.al. [Braun 04a, Briggs 01] have proposed a similar solution to the problem, but 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" operator 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. `Quantum mechanics typically depicts physical reality as a vector in Hilbert space at a distinct point in time, with Schrödinger's equation governing its progression. This equation features an externally imposed time parameter, which can be problematic if the universe is viewed as a quantum mechanical system. This is because there shouldn't be any external time in such a system.` 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 involv-

ing 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]

[Mendes 19] Has a very nice introduction to the approach, especially the Page1 column 2, first paragraph

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[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

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

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

The total wave function Ψ can be written as

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

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

Where $\{\psi' s\}$ represent the energy eigenstates of $H_{\mathcal{S}} + H_{\mathcal{S}\mathcal{E}}$ at a fixed R, with $\epsilon_n(R) = \langle \psi_n | H_{\mathcal{S}} + H_{\mathcal{S}\mathcal{E}} | \psi_n \rangle$, 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

$$H_{\mathcal{E}} = K + V_{\mathcal{E}}(R). \tag{2.3}$$

with:

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

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]:

$$\sum_m \langle \psi_n | \left(\frac{-\hbar^2}{2M} \nabla_R^2 \right) | \psi_m \rangle \chi_m(R) + V_{\mathcal{E}}(R) \chi_n(R)$$
$$+ \sum_m \langle \psi_n | H_{\mathcal{S}} + H_{\mathcal{S}\mathcal{E}} | \psi_m \rangle \chi_m(R) = E \chi_n(R). \tag{2.5}$$

The "potentials":

$$\mathcal{V}_{mn}(R) = \langle \psi_m | H_{\mathcal{S}} + H_{\mathcal{S}\mathcal{E}} | \psi_n \rangle. \tag{2.6}$$

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

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

We define

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

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

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

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.

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[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

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

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, i.e., we neglect the off-diagonal terms.

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

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

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:

$$\frac{d\boldsymbol{P}_n}{dt} = -\nabla_{R_n} H = \nabla_{R_n} (V_{\mathcal{E}}(R) + E_n(R)) \quad (2.15)$$

$$\frac{d\boldsymbol{R}_n}{dt} = \nabla_{P_n} H. \quad (2.16)$$

For the standard kinetic energy $\frac{P^2}{2M}$, 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

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

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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

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

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

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

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

$$\nabla_R W = M \frac{d\boldsymbol{R}}{dt} \quad (2.21)$$

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:

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

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 $\mathrm{H}_{\mathcal{S}\mathcal{E}}$

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]

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

Where λ is any complex-valued parameter, $\mathbf{H}$ 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)

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

For our analysis, we assume that λ 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

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

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

$$\langle \chi_0 | e^{i\lambda(\mathbf{H}-E)} |\Psi\rangle\rangle = \langle \chi_0 | \Psi\rangle\rangle$$
$$\langle \chi_0 | e^{i\lambda(\mathbf{H}_c-E)} |\Psi\rangle\rangle = e^{-i\lambda\mathbf{H}_s} \langle \chi_0 | \Psi\rangle\rangle . \tag{3.3}$$

We define

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

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,

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

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

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

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 $A_c(\lambda) \equiv \langle \chi_\lambda | \mathbf{A}_c |\chi_\lambda\rangle$. An ideal choice would be to use such a $\mathbf{A}_c$ 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.

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[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., $\mathbf{V} = \mathbf{0}$. However, in real scenarios, one always has some interaction within components of a global closed system. To extend the derivation to non-zero $\mathbf{V}$, we modify our clock state as

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

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

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

We can rearrange the above equation to write it as

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

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

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

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

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

Using above defined operators, we decompose the

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

where

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

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

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

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 $\mathcal{H}$.

3.1 Example: Dynamics of two interacting (1/2)-spins

Coefficient of the system's state $|\psi\rangle$
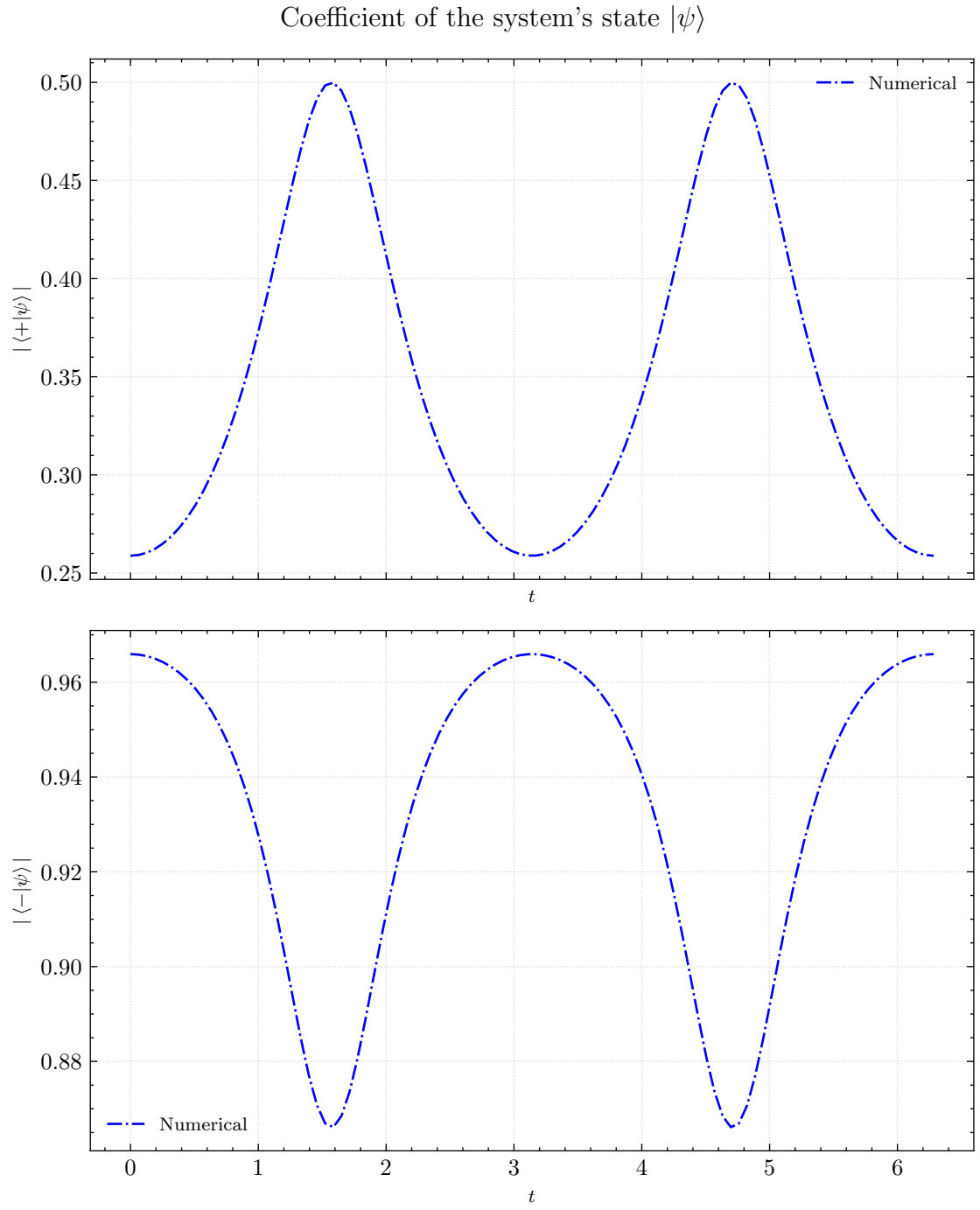

Figure 3.1: Two interacting (1/2)-spins

Components of the system's emergent potential $V_s(\lambda)$
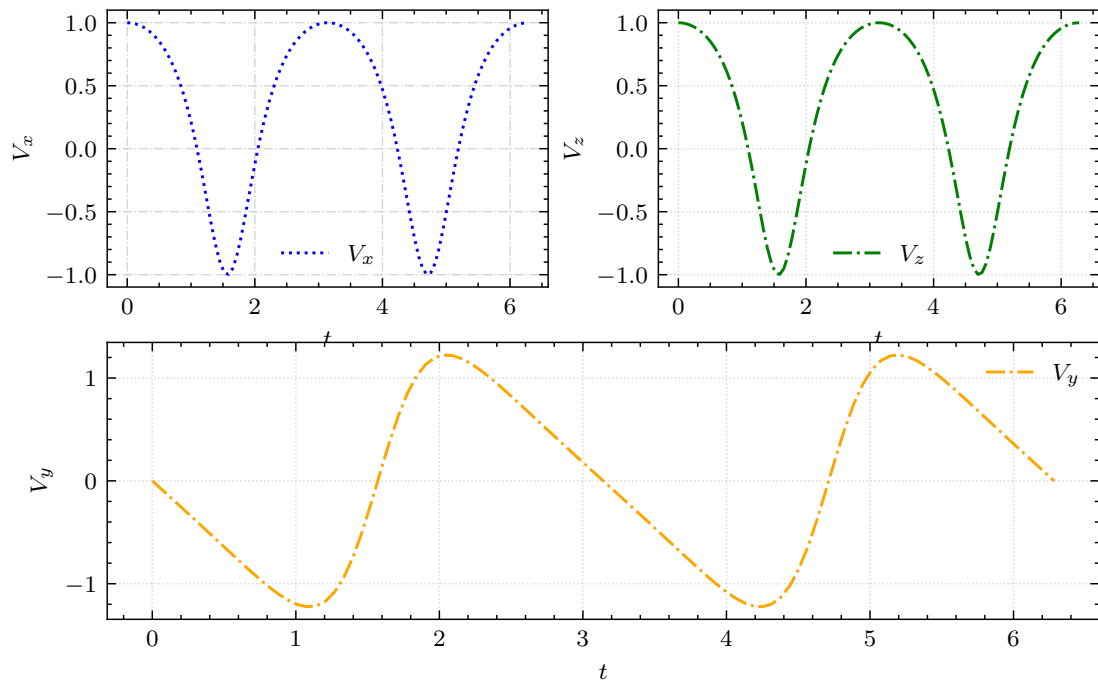
Figure 3.2: Two interacting (1/2)-spins

Chapter 4

Semi-Classical Relational Dynamics for Light-Matter Interaction

It has been shown in Chapter 2 how one can reduce a TISE to a TDSE for a system in the presence of a classical environment. In this chapter, we will discuss the application of the previous chapter to a simple model of light-matter interaction and enumerating the conditions that must be obtained in order to treat the electromagnetic field classically. The upcoming sections outlines the derivations as presented in [Braun 04b].

To get the time-dependence, we start by considerig a time-independent hamiltonian of an interacting quantum system, with a Hamiltonian given as

$$H = H_s(p, x) + H_F(P, Q) + H_I(x, Q). \tag{4.1}$$

where (x, p) and (Q, P) are (position, momentum) operator for system and boson field, respectively. Also, H_s is the Hamiltonian of the atomic system, H_F is the field hamiltonian, and H_I is the interaction hamiltonian. The boson field hamiltonian will be takes a sum over field modes, with hamiltonian given as

$$H_F(P, Q) = \sum_k \frac{1}{2} \left(P_k^2 + \omega_k^2 Q_k^2 \right) \tag{4.2}$$

We write the above Hamiltonian in terms of creating and annihilation operators

$$H = \sum_i \epsilon_i c_i^\dagger c_i + \sum_k \hbar \omega_k \left(a_k^\dagger a_k + \frac{1}{2} \right) + \hbar \sum_k g_{jk}^k c_i^\dagger c_i \left(a_k^\dagger + a_k \right). \tag{4.3}$$

where c_i and $c_i^\dagger$ are the annihilation and creation atomic operators for the system, and a_k and $a_k^\dagger$ are the annihilation and creation operators for the boson field.

A special case of the above Hamiltonian is when we take a two level atom (or a spin 1/2 system) interacting with a single mode of the electromagnetic field. Eqn. 4.3 then reduces to

$$H = \hbar\omega_0\sigma_z + \hbar\omega\left(a^\dagger a + \frac{1}{2}\right) + \hbar g\sigma_x\left(a + a^\dagger\right), \tag{4.4}$$

where σ_z and σ_x are the Pauli matrices. This special case is known as the Jaynes-Cummings model.

4.1   Semiclassical limit of the JC-Model

As done in Eqn. 2.2, one can write in general the solution of TISE

$$(H - E)\Psi = 0 \tag{4.5}$$

with H in the form of Eqn. 4.3 as

$$\Psi(x, Q) = \sum_k \chi_k(Q)\phi_k(x, Q). \tag{4.6}$$

We employ this particular form, wherein $\chi_k(Q)$ displays no reliance on x, under the assumption that the system exerts minimal back-reaction on the field. This assumption has been utilized previously in Chapter 2 and will be employed again in forthcoming derivations.

Doing the same exercise as in Eqn. 2.5, we substitute Eqn. 4.6 into Eqn. 4.5 and obtain a set of coupled equations

$$\sum_i \chi_i(Q)\left[H_s + H_I - \left(E - \sum_k \frac{1}{2}\omega_k^2 Q_k^2 + \frac{\hbar^2}{2\chi_i}\frac{\partial^2}{\partial Q_k^2}\chi_i\right)\right]$$

$$+ \sum_i \chi_i(Q)\left[\frac{-\hbar^2}{2}\frac{\partial^2}{\partial Q_k^2} - \frac{-\hbar^2}{\chi_i}\frac{\partial}{\partial Q_k}\chi_i\frac{\partial}{\partial Q_k}\right]\phi_i(x, Q) = 0. \tag{4.7}$$

Eqn. 4.7 when projected onto state ϕ_j gives

$$\sum_k \left[-\frac{\hbar^2}{2}\frac{\partial^2}{\partial Q_k^2} + \frac{1}{2}\omega_k^2 Q_k^2\right]\chi_j + \sum_i \langle\phi_j|\, H_s + H_I\, |\phi_i\rangle\,\chi_i$$

$$- \sum_{i,k}\left[\langle\phi_j|\,\frac{\hbar^2\partial^2}{2\partial Q_k^2}\,|\phi_i\rangle + \langle\phi_j|\,\hbar^2\frac{\partial}{\partial Q_k}\,|\phi_i\rangle\frac{\partial}{\partial Q_k}\right]\chi_i = E\chi_j. \tag{4.8}$$

The equation above describes the "close-coupled" form for χ_j. The off-diagonal terms account for changes in the state of the boson field caused by changes in

the system's state. Neglecting these off-diagonal coupling terms simplifies the equation, providing the state of χ_j when the system is in state ϕ_j, i.e.,

$$\left[\sum_k \left(-\frac{\hbar^2}{2} \frac{\partial^2}{\partial Q_k^2} + \frac{1}{2}\omega_k^2 Q_k^2 \right) + E_j(Q) - E \right] \chi_j$$
$$= \hbar^2 \sum_k \langle \phi_j | H_s + H_I | \phi_j \rangle \frac{\partial}{\partial Q_k} \chi_j. \tag{4.9}$$

with

$$E_j(Q) = \langle \phi_j | H_s + H_I - \sum_k \frac{\hbar^2}{2} \frac{\partial^2}{\partial Q_k^2} | \phi_i \rangle. \tag{4.10}$$

The diagonal $\langle \phi_j | H_s + H_I | \phi_j \rangle$ terms on the RHS of Eqn. 4.9 are zero for real ϕ_j or else can be eliminated by a (Berry) phase transformation [Braun 04b]. In addition, since we are neglecting the first order derivatives w.r.t. Q_k, it's consistent to neglect the second order derivatives as well, which gives us the following equation

$$\left[\sum_k \left(-\frac{\hbar^2}{2} \frac{\partial^2}{\partial Q_k^2} + \frac{1}{2}\omega_k^2 Q_k^2 \right) + E_j(Q) - E \right] \chi_j(Q) = 0. \tag{4.11}$$

this is the defining equation for the state of the boson field when the system is in state ϕ_j.

For, complete independence of the field from the system, we need to replace $E_j(Q)$ by some fixed average energy $\bar{E}(Q)$ and corresponding $\chi_j(Q)$ by some "mean"-field state $\chi(Q)$. Hence, we replace

$$\chi_j(Q) = a_j(Q)\chi(Q). \tag{4.12}$$

where we assume $a_j(Q)$ to be slowly varying function of Q. The Eqn. 4.6 reduces to

$$\Psi(x, Q) = \chi(Q) \sum_j a_j(Q)\phi_j(x)$$
$$\Psi(x, Q) = \chi(Q)\psi(x, Q). \tag{4.13}$$

We've identified the key approximations needed to express the exact wave function (Eqn. 4.6) in the simpler, factorized form (Eqn. 4.13). This step is critical because it assumes the influence of the atom on the field is minimal, while the field has a strong influence on the atom. Now, we can focus on deriving the effective Schrödinger equation for the wave function (denoted by ψ) representing the quantum system.

Note that, one can in general, view Eqn. 4.13 as a general ansatz for the wave function and find from Eqn. 4.5[1]

$$(H - E)\Psi = \chi(Q) \left[H_S + H_I(x, Q) - \frac{\hbar^2}{2} \left(\frac{\partial^2}{\partial Q^2} + 2\frac{\chi'(Q)}{\chi(Q)} \frac{\partial}{\partial Q} \right) \right] \psi(x, Q)$$

$$+ \psi(x, Q) \left[-\frac{\hbar^2}{2} \frac{\partial^2}{\partial Q^2} + \frac{\omega^2}{2} Q^2 - E \right] \chi(Q) = 0 \tag{4.14}$$

To streamline our analysis, we'll now focus on a single field mode. This derivation takes a slightly different approach compared to both the method outlined in Chapter 2 and the one we'll use later for the Jaynes-Cummings model (our toy model universe). We present this alternative approach to lay the groundwork for the new considerations in the next section, which will leverage coherent states.

We split the action of the total Hamiltonian on the field ad quantum system such that the wave function $\chi(Q)$ described the field with energy close to total energy E, while the reaming part of the equation describes the quantum system (with negligible energy in camparison). Completely ignoring the influence of the quantum system on the field (back coupling) is analogous to neglecting the terms $\bar{E}(Q)$ in the equations. This simplification allows us to select a wave function for the field, which will ultimately be treated classically. This is equivalet to neglecting $\bar{E}(Q)$ and allows one to choose the wave function of the field which is to become classical, This wave function must be an eigenstate of the fixed-field Schrödinger equation , i.e.

$$\left[\sum_k \left(-\frac{\hbar^2}{2} \frac{\partial^2}{\partial Q_k^2} + \frac{1}{2}\omega_k^2 Q_k^2 \right) - E \right] \chi(Q) = 0. \tag{4.15}$$

Under the assumption of these large (classical) energies and assuming we're sufficiently far from any classical turning points, we can approximate the actual wave function, denoted by $\chi(Q)$, by its WKB approximation, i.e.,

$$\chi(Q) = \exp \left(\frac{i}{\hbar} \int^Q dQ' P(Q') \right). \tag{4.16}$$

where $P(Q)$ is the momentum of the field, given as

$$P(Q) = \sqrt{2 \left(E - \frac{1}{2}\omega^2 Q^2 \right)}. \tag{4.17}$$

Using Eqn. 4.14 - Eqn. 4.16 gives

$$\left[\sum_k \left(-\frac{\hbar^2}{2} \frac{\partial^2}{\partial Q_k^2} + \frac{1}{2}\omega_k^2 Q_k^2 \right) - E \right] \exp \left(\frac{i}{\hbar} \int^Q dQ' P(Q') \right) = 0$$

$$\left[H_s + H_I(x, Q) - \frac{\hbar^2}{2} \frac{\partial^2}{\partial Q^2} - i\hbar P(Q) \frac{\partial}{\partial Q} \right] \psi(x, Q) = 0. \tag{4.18}$$

---

[1]Here we assumed only single mode of E.M field

The above differential equation describes the dynamics of (atomic part) the quantum system. We simplfy this equation by replacing the equation by a parameter t, which parametrizes $Q(t)$ trajectory and define

$$P(Q)\frac{\partial}{\partial Q} \equiv \frac{\partial}{\partial t} \tag{4.19}$$

It's evident that $P(Q)$ derived from Eqn. 4.17 corresponds to the velocity $\dot{Q}$, as dictated by classical equations of motion. These equations state that $\dot{Q} = P$ and $\dot{P} = -\omega^2 Q$, where $Q(t) = Q_0 \cos(\omega t)$ represents *the solution, demonstrating that the parameter t signifies classical time.*

We define $\psi(x,t) = \psi(x, Q(t))$ and find from Eqn. 4.18

$$i\frac{\partial}{\partial t}\psi(x,t) = \left[H_s + H_I(x, Q(t))\frac{\hbar^2}{2}\left(\frac{\ddot{Q}(t)}{\dot{Q}^3(t)}\frac{\partial}{\partial t} - \frac{1}{\dot{Q}^2(t)}\frac{\partial^2}{\partial t^2}\right)\right]\psi(x,t). \tag{4.20}$$

The derivatives appearing on the right-hand side stem from the second-order derivative $\frac{\partial^2}{\partial Q^2}$ wrt position, when expressed in terms of time derivatives. In the scenario of a substantial ("classical") amount of energy E, predominantly residing in the classical degree of freedom Q, these additional terms become negligible, as we will soon illustrate. Initially, it's worth noting that $\frac{\partial}{\partial t}$ is of the order of energy of the quantum system, $E_s = \langle H_s + H_I \rangle$, implying it is considerably smaller than E. This allows us to disregard the supplementary derivative terms on the right side of Eqn. 4.20. Proceeding with self-consistency, and leveraging $\dot{Q} = P \approx \sqrt{E}$ for the harmonic oscillator away from its turning points, as well as $\ddot{Q} \approx \omega \dot{Q}$, we can estimate their respective orders of magnitude. First,

$$\left\langle\frac{\hbar^2}{2}\frac{\ddot{Q}(t)}{\dot{Q}^3(t)}\frac{\partial}{\partial t}\right\rangle \approx E_s\frac{\hbar\omega}{E}, \text{ and } \left\langle\frac{\hbar^2}{2}\frac{1}{\dot{Q}^2(t)}\frac{\partial^2}{\partial t^2}\right\rangle \approx \frac{E_s^2}{E^2}. \tag{4.21}$$

The additional derivative terms on the right-hand side of Eqn. 4.20 exhibit an order of magnitude of $E_s\left(\frac{E_s+\hbar\omega}{E}\right)$. Hence, in comparison to the remaining terms on the right-hand side, which are of the order E_s, these additional terms are diminished by a factor approximately $\frac{\hbar\omega}{E} \approx \frac{1}{n}$, where n represents the number of photons in the field mode. This factor is significantly small for a classical field. Hence, we can neglect these terms and write

$$i\frac{\partial}{\partial t}\psi(x,t) = [H_s + H_I(x, Q(t))]\psi(x,t) \tag{4.22}$$

which is the usual form of TDSE for the quantum system interacting with the classical field.

The derivation relies on the Time-Independent Schrödinger Equation (TISE) for both the atom and the field. Time arises as a consequence of classical motion,

serving solely as a derived classical parameter. It's important to note that the aforementioned arguments hold true only away from turning points where the velocity $\dot{Q}(t)$ is non-zero. But it's evident that the Time-Dependent Schrödinger Equation (TDSE) of (Eqn. 4.22) remains valid for all times. The reason behind this limitation is apparent: it lies in the selection of Q, the position representation, for the field mode. While this choice aids in diagonalizing the coupling Hamiltonian H_I, in this representation, the real field quadrature $Q(t)$ undergoes harmonic motion with periodic zeros in its time derivative $\dot{Q}(t)$. Consequently, the position representation fails to offer a global notion of time. Next section will illustrates how this limitation can be addressed by utilizing a coherent state representation of the field state.

4.2 Coherent State Derivation of TDSE

In quantum optics, coherent states hold a special place. Representing minimal uncertainty in both position (Q) and momentum (P) of the field mode, these states exhibit classical behavior. It's therefore unsurprising that coherent states play a crucial role in deriving a time-dependent Schrödinger equation for the quantum system's degrees of freedom. This derivation leverages a time-independent Schrödinger equation encompassing both the coupled quantum system and the field mode.

We begin by writing the total hamiltonian for single mode of E.M field in term of usual creation and annihilation operators as

$$
\begin{aligned}
\mathbf{H}_F &= \hbar\omega\left(\mathbf{a}^\dagger\mathbf{a} + 1/2\right), \\
\mathbf{H}_I &= \hbar\mathbf{S}(\mathbf{a} + \mathbf{a}^\dagger)
\end{aligned}
\tag{4.23}
$$

with $\mathbf{S} = \sum_{ij}^k g_{ij}\mathbf{c}_i^\dagger\mathbf{c}_i$ as in Eqn. 4.3.

Coherent state, defined as, $|\alpha\rangle = \exp\left(|\alpha|^2/2 + \alpha\mathbf{a}^\dagger\right)|0\rangle$ where α is a complex number, is an eigenstate of the annihilation operator, i.e., $\mathbf{a}|\alpha\rangle = \alpha|\alpha\rangle$. Some crucial properties that will be of use to us are

$$
\begin{aligned}
\langle\alpha|\mathbf{a}^\dagger &= \alpha^*\langle\alpha|, \\
\langle\alpha|\mathbf{a} &= \left(\frac{\partial}{\partial\alpha^*} + \frac{\alpha}{2}\right)\langle\alpha|.
\end{aligned}
\tag{4.24}
$$

Coherent states form an overcomplete basis, i.e., any state $|\psi\rangle$ can be expanded as

$$
|\psi\rangle = \int\frac{d^2\alpha}{\pi}|\alpha\rangle\langle\alpha|\psi\rangle \equiv \int\frac{d^2\alpha}{\pi}|\alpha\rangle\tilde{\chi}(\alpha, \alpha^*).
\tag{4.25}
$$

where $\tilde{\chi}(\alpha, \alpha^*) = \langle \alpha | \psi \rangle$. Note that we can always write

$$\tilde{\chi}(\alpha, \alpha^*) = \chi(\alpha^*) \exp\left(-|\alpha|/2\right)$$

where $\chi(\alpha, \alpha^*)$ is a complex function of α. Instead of utilizing the position Q representation as previously done, we leverage the properties of coherent states mentioned above to express the Time-Independent Schrödinger Equation (TISE) within the coherent state representation relative to the classical degree of freedom. We write the total wave function

$$\langle \alpha | \Psi \rangle = \exp\left(-|\alpha|^2/2\right) \chi(\alpha^*) \psi(\alpha^*). \tag{4.26}$$

As before, we will consider $\exp\left(-|\alpha|^2/2\right) \chi(\alpha^*)$ to describe the classical degree of freedom, while $\psi(\alpha^*)$ will represent the quantum system without backreaction to the classical degree of freedom.

Another important property of the conherent state is it's overlap with the photon number state, which is given as $\langle n | \alpha \rangle = \exp\left(-|\alpha|/2\right)(\alpha^*)^n/\sqrt{n!}$. In the limit of large photon number n, it's easy to see that only those coherent states $|\alpha\rangle$ with

$$|\alpha|^2 = n \tag{4.27}$$

will contribute significantly to the number state $|n\rangle$.

Another significant property of coherent states is their overlap with photon number states, expressed as $\langle n | \alpha \rangle = \exp\left(-|\alpha|/2\right)(\alpha^*)^n/\sqrt{n!}$. When considering a large photon number n, it becomes evident that only coherent states $|\alpha\rangle$ satisfying the condition:

$$|\alpha|^2 = n \tag{4.28}$$

contribute significantly to the corresponding number state $|n\rangle$. With Eqn. 4.26 in mind, the TISE with H_F and H_I from Eqn. 4.25 now reads

$$\langle \alpha | (H - E) | \Psi \rangle = \chi(\alpha^*) \left[H_s + \hbar g \left(\alpha^* + \frac{\chi'(\alpha^*)}{\chi(\alpha^*)} + \frac{\partial}{\partial \alpha^*} \right) \sigma_x + \hbar \omega \alpha^* \frac{\partial}{\partial \alpha^*} \right] | \psi(\alpha^*) \rangle$$

$$+ | \psi(\alpha^*) \rangle \left[\hbar \omega \left(\alpha^* \frac{\partial}{\partial \alpha^*} + \frac{1}{2} \right) - E \right] \chi(\alpha^*) = 0. \tag{4.29}$$

The above equation corresponds to Eqn. 4.14 of position space approach. Just as we did in Section 4.1, we chose χ to be an eigenstate of the field Hamiltonian, i.e., to be a number state $|n\rangle$ with energy $E = \hbar \omega [n + 1/2]$. In coherent state representation,

$$\chi(\alpha^*) = (\alpha^*)^n/\sqrt{n!}. \tag{4.30}$$

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This ensures that the second part of Eqn. 4.29 dissappears and one notices that

$$\frac{\chi'(\alpha^*)}{\chi(\alpha^*)} = \frac{n}{\alpha^*} = \frac{\alpha^*\alpha}{\alpha^*} = \alpha. \tag{4.31}$$

Using Eqn. 4.30 and Eqn. 4.31 in Eqn. 4.29 gives

$$\left[H_s + \hbar S\left(\alpha^* + \alpha + \frac{\partial}{\partial\alpha^*}\right) + \hbar\omega\alpha^*\frac{\partial}{\partial\alpha^*}\right]|\psi(\alpha^*)\rangle = 0. \tag{4.32}$$

We now introduce a new parameter t, which replaces α analogous to what we did in position space representation. The parameter t is defined through a complex trajectory $\alpha^*(t)$ for the coherent state field amplitude, such that

$$\hbar\omega\alpha^*\frac{\partial}{\partial\alpha^*} \equiv -i\hbar\frac{\partial}{\partial t}. \tag{4.33}$$

Hence, time is determined by the classical motion of the field amplitude, which in this case is

$$\alpha(t) = \alpha_0 e^{-i\omega t}. \tag{4.34}$$

Importantly, whereas the position space expression (Eqn. 4.19) becomes problematic near classical turning points due to $P(Q) = 0$, the coherent state expression (Eqn. 4.33) maintains finiteness throughout all times. Furthermore, it's noteworthy that the coherent state equation (Eqn. 4.32) exclusively involves first-order derivatives. This characteristic closely resembles the first-order time-dependent Schrödinger equation, whereas the position space expression (Eqn. 4.20) is of second order.

We see that the field part of the interaction Hamiltonian becomes,

$$\left[\alpha^* + \alpha - \alpha\left(\hbar\omega|\alpha|^2\right)^{-1}(i\hbar\partial/\partial t)\right] \tag{4.35}$$

In large photon number limit $1/|\alpha|^2 \approx 1/n$, vanishes. This can be compared to the similar discussion after Eqn. 4.20. Therefore we find that, in the limit of large photon number, the TDSE for state $|\psi(t)\rangle$ is

$$i\hbar\frac{\partial}{\partial t}|\psi(t)\rangle = \left[H_s + \hbar S\left(\alpha_0 e^{-i\omega t} + \alpha_0 e^{i\omega t}\right)\right]|\psi(t)\rangle. \tag{4.36}$$

Under the assumption of a valid two-level approximation, the system can be represented by the operator $S = g\sigma_x$. Crucially, unlike the equivalent result obtained in position space representation, the derivation of Eqn. 4.36 using coherent states is valid for all times.

Furthermore, this equation for a two-level system interacting with a single electromagnetic field mode is of critical importance. We will leverage it to compare the system's dynamics obtained through this approach to those obtained from a fully quantum relational dynamics approach in the next section.

Chapter 5

Quantum Relational Dynamics of Jaynes–Cummmings Model

In Chapter 4, we delved into the semi-classical approach for deriving the Time-Dependent Schrödinger Equation (TDSE) governing the Jaynes-Cummings model. This method assumes a semi-classical (WKB-like) wave function for the field mode. However, this approach inherits the concept of "time" as a purely classical parameter, thereby compromising its deeper, more fundamental nature.

In contrast, in 3, we presented a purely quantum framework for describing the dynamics of general interacting system. Here, "time" emerges as a symmetry parameter stemming from the principle of global invariance of the global energy eigenstate of total Hamiltonian.

This chapter explores the Jaynes-Cummings model from the perspective of Quantum Relational Dynamics.. We aim to scrutinize the transition from a purely quantum system to semi-classical regimes, as previously discussed in Chapter 4, and to juxtapose the dynamics as characterized by the two distinct approaches.We demonstrate that, under appropriate limits (consistent with the semiclassical treatment), the two approaches yield identical results. Interestingly, the analysis also hints at the presence of a superselection rule.

We assume a special

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 (Noether's 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 $t \rightarrow t(\tau)$ i.e to a dynamical variable. In terms of τ the action

(Eqn. A.1) can be expressed as:

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

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]:

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

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

Let's calculate the conjugate momenta:

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

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

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

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

We have:

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

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

$$\boxed{H = 0} \qquad \text{(A.7)}$$

Therefore, for parameterization-invariant theory, the Hamiltonian function is identically zero. It is crucial to note that this *derivation makes no assumptions*

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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 $\mathbf{J}$, which we call the superselection charge. If a self-adjoint operator $\mathbf{A}$ represents a measurable quantity, it must satisfy the commutativity [Tanimura 11]

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

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

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

where $\mathbf{H}$ is the Hamiltonian $\mathbf{H}$ of the system. The conservation law (Eqn. B.3) requires that $\mathbf{J}$ commutes with the Hamiltonian $\mathbf{H}$ while the superselection rule (Eqn. B.2) requires that $\mathbf{J}$ commutes with all of the measurable quantities. Thus, the superselection rule is a stronger requirement for $\mathbf{J}$ 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 $\mathbf{A}$ and any eigenvector $|\psi_i\rangle$ of $\mathbf{J}$ with charge q_i[1].

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

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

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

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 $\mathbf{J}$ is non degenerate

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