Decoherence
and
the quantum-to-classical transition

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by

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CERTIFICATE

This is to certify that the project titled **Decoherence and the quantum-to-classical transition** is a bona fide record of work done by **Mohammad Asif Azad** (PH16C021) towards the partial fulfillment of the requirements of the Master of Science degree in Physics at the Indian Institute of Technology, Madras, Chennai 600036, India.

(L. Sriramkumar, Project supervisor)

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ABSTRACT

The behavior of open quantum systems has attracted considerable attention over the years and these studies have revealed that the interaction between the system and environment is key to unraveling how this classical world arises from the essentially non-intuitive principles of quantum mechanics. Decoherence provides us answers about why we see classical particles in definite positions, for instance, instead of a superposition of them and it seeks to explain how certain variables of the system are preferred over others in terms of showing classical behavior at the system level even when the dynamics of the combined environment-system is essentially quantum. In this piece of work, after providing the motivation behind the search for a theory of open quantum systems and a brief introduction to the theory, we try to apply it to simple open quantum systems to bring out the prime implications of the theory. We also rederive the results of a classic paper by Unruh and Zurek on decoherence in a model of quantum Brownian motion.

Contents

Chapter 1

Contrasting quantum and classical: a short review of concepts and tools

1.1 Introduction

The view of the physical world as offered by classical mechanics was very intuitive, as it corresponded to our direct experience. The advent of quantum mechanics altered this world view drastically, and in many ways that are quite non-intuitive. But out of all the ways in which quantum mechanics differs from classical mechanics, perhaps the most poignant one is its departure from the latter in terms of the description, and possibilities, of a physical system. Instead of describing a system in terms of individual position and momenta $\{x_i, p_i\}$ and their functions, quantum mechanics, in its most standard formulation, describes it by a state vector in an abstract Hilbert space. The fact that a superposition of such states is also a valid physical state lies at the heart of most of the surprising predictions of quantum mechanics . In this chapter, we shall try to introduce the reader to some of these predictions and ask why such effects are not so much visible at the macroscopic scale . Then we shall try to convince the reader that the causes of the classical behavior of systems can be traced back to interactions with the environment . After that, we shall introduce certain tools that will enable us to study open quantum systems before delving into a formal study of open quantum systems in the next chapter.

1.2 The superposition principle

Let $\{|\psi_n\rangle\}$ be a set of physical quantum states of a system. Then according to the superposition principle of quantum mechanics [2]

$$|\Psi\rangle = \sum_n c_n |\psi_n\rangle \tag{1.1}$$

is also a valid physical quantum state for the system for arbitrary complex coefficients c_n. (Following the standard textbook formulation, one may impose the normalization $\sum_n |c_n|^2 = 1$ to make it a normalized state.) For example, if $|0\rangle$ and $|1\rangle$ respectively represent the spin-up and spin-down states of a spin-$\frac{1}{2}$ particle, then

$$|\psi\rangle = \frac{1}{\sqrt{2}}(|0\rangle + |1\rangle) \tag{1.2}$$

is also a valid spin state of the particle. We shall use the example of a superposition of two position states to show the meaning and non-trivial implications of the superposition principle.

1.2.1 The double-slit experiment

In the double-slit experiment, we permit a beam of electrons pass through two slits and observe the pattern on a distant screen. Let us name the slits as, 1 and 2. First, we close slit 2 and fire the electron beam at the slits. The electrons that come out on the other side, disregarding for the time being the very interesting phenomenon of quantum tunneling, must have gone then through slit 1. Let us denote by $|\psi_1\rangle$ the state of the electron after passing thus through slit 1. Analogously, we keep slit 2 open and close slit 1 to obtain the electron in state $|\psi_2\rangle$. Now if the electron is described by $|\psi_i\rangle$, i.e. it passed through the ith slit, then the probability density distribution of the electron at the screen, $\rho(x)$ will be given by

$$\rho(x) = \left|\langle x|\psi_i\rangle\right|^2 = \left|\psi_i(x)\right|^2. \tag{1.3}$$

If we assume that each electron passed through either one of the slits, then the density distribution should have been given by

$$\rho(x) = \left|\langle x|\psi_1\rangle\right|^2 + \left|\langle x|\psi_2\rangle\right|^2 = \left|\psi_1(x)\right|^2 + \left|\psi_2(x)\right|^2, \tag{1.4}$$

where we are just adding the density distributions of the electrons coming through each slit. But we observe that the density distribution is found to be

$$\rho(x) = \frac{1}{2}\big|\psi_1(x)\big|^2 + \frac{1}{2}\big|\psi_2(x)\big|^2 + \mathrm{Re}\{\psi_1(x)\psi_2^*(x)\} = \frac{1}{2}\big|\langle x|\psi_1\rangle + \langle x|\psi_2\rangle\big|^2 \, , \qquad (1.5)$$

which means that the state of the electrons after passing through the slits must be described by

$$|\psi\rangle = \frac{1}{\sqrt{2}}(|\psi_1\rangle + |\psi_2\rangle) \, . \qquad (1.6)$$

A superposition such as Eq. (1.6) does not represent the state of a particle which "actually" went through either one of the slits 1 or 2 with equal probabilities, nor does it refer to the limitation in our knowledge about which slit the electron went through . Rather Eq. (1.6) contains all the information that can be known about the system and describes a state in which both the components are simultaneously present at all times .

Conclusion: This example beautifully presents the implications and meaning of the statement that a superposition of physically realizable states can also be a valid physical state in standard quantum mechanics. In this example, the electron, at the level of the slits, is simultaneously present at two distinct positions (slits) - a very non-classical state of affairs. Also, the coherence between the components $\psi_1(x)$ and $\psi_2(x)$ in the state $\psi(x)$ given by Eq. (1.6) is represented by the interference term, $\mathrm{Re}\{\psi_1(x)\psi_2^*(x)\}$, in Eq. (1.5).

1.2.2   Observability of interference effects at macroscopic level

In the previous section, we discussed how superposition effects are easily visible at the sub-atomic scales. But as we go on to macroscopic scales, such interference effects, which reveal the quantum nature of systems, become really difficult to observe. In the usual textbook study of quantum mechanics, the unobservability of interference phenomena at macroscopic level is associated with our inability to experimentally probe scales which are necessary to resolve such patterns. For example, the wavelength λ associated with the matter wave of a particle of mass m moving with a velocity v is typically given as the de Broglie wavelength:

$$\lambda = \frac{h}{mv} \, , \qquad (1.7)$$

where h is the Planck's constant .

For a particle of mass 1 gm moving with a velocity of 1 m/s, this wavelength equals

6.626×10^{-29} cm which is too small to be resolved with the current experimental techniques .
But what is often neglected while answering these questions is the fact that the environment
starts becoming ever more important as we increase the size of the system.

Not only that , recent experiments have been able to create these interference patterns with
molecules as large as C_{70} and they have revealed that these interference patterns start dis-
appearing as we keep increasing the rate of environmental interaction. To emphasize the
importance of the environmental interaction in the disappearance of interference patterns
and hence in the loss of quantum behavior of systems, we shall discuss a recent experi-
ment which studied the effect of environment on the interference pattern created by C_{70}
molecules.

1.2.3 Interferometry with C_{70} molecules and decoherence

We have already seen how interference effects were observed in double-slit experiments with electrons and discussed, in the previous section, the difficulty of observing interference effects for macroscopic objects. But recent advances in experimental methods have enabled experimentalists to observe interference effects in molecules having a mass exceeding *10000 amu* and containing more than *810 atoms* [6]. Here we shall discuss an experiment carried out by Hackermüller et al. [7] which showed the existence of interference effects with C_{70} molecules and suppression of interference due to interaction with gas molecules in the setup. One C_{70} molecule is almost *seven hundred thousand times heavier* than an electron.

Figure 1.1: Decrease of interference effects from the left panel to the right panel due to an increase of surrounding air pressure. The x-axis is the position of the third grating in the experiment, which acts as a mask that is moved transverse to the beam and in front of the detector to measure the interference pattern produced by the first two gratings. [Figure taken from [7]]

The de Broglie wavelengths were of the order of a few picometers with the velocities employed, but the experimentalists employed some clever techniques to observe the interfer-

ence with even such minute de Broglie wavelengths (see [11], Section 6.2 for a brief discussion of the experimental procedure). But what is important for our discussion is the fact that they were able to observe a reduction in the strength of interference when the gas pressure in the experimental setup was increased. This fits in neatly into the paradigm of decoherence since an increase in gas pressure will increase the interaction of the C_{70} molecules with the gas molecules and the increased environmental interaction leads to increased decoherence. This variation is visible in Fig. 1.1. In fact, these experimentalists were able to study the gradual decrease of interference effects with the increase of air pressure by defining a quantity called *visibility* $V(p)$ by

$$V(p) = \frac{c_{max}(p) - c_{min}(p)}{c_{max}(p) + c_{min}(p)} , \tag{1.8}$$

where $c_{max}(p)$ and $c_{min}(p)$ are the maximum and minimum amplitudes, respectively, at pressure p. For a perfect interference pattern, $c_{min}(p) = 0$ and hence $V(p) = 1$. For no interference at all, $c_{min}(p) = c_{max}(p)$ giving rise to $V(p) = 0$. The experimentalists increased the air pressure gradually and found out that visibility decreased linearly with the increase in air pressure. This variation is shown in Fig. 1.2.

These experiments indicate the trend of observing interference effects in bigger and bigger objects, and it seems increasingly likely that we might be able to produce interference effects between objects large enough to be visible to the naked eye. But what is even more interesting is the fact that we now have definite proof that environmental interaction plays a major part in the loss of coherence of quantum states. Motivated by such results, we shall set out to study the theory of open quantum systems and learn some of the necessary tools in the next few sections.
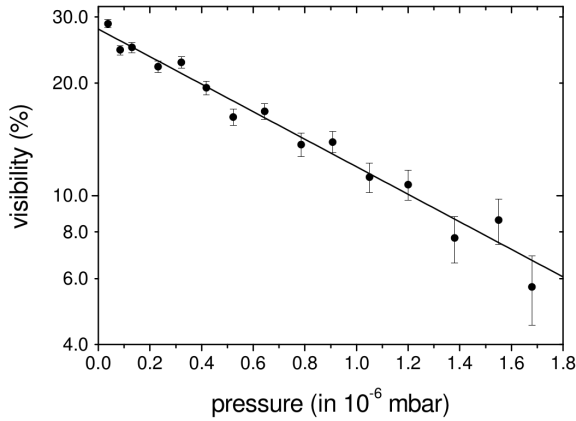

Figure 1.2: Decrease of visibility of the interference pattern with increasing air pressure. [Figure taken from [7]]

1.3 Open quantum systems: necessary tools

In the previous section, we saw an experiment that showed us how environmental interaction can affect the dynamics of a system and renders its quantum properties unobservable. This is one of the motivations for us to study open quantum systems to see if we can get a quantitative measure of the environment's effect on the properties of the system. But such a study in the framework of quantum mechanics necessitates a familiarity with certain tools and concepts, such as entanglement, density matrices, Wigner functions, etc. So, before going to the study of open quantum systems in the next chapter, we shall discuss these tools in the subsequent sections.

1.4 Entanglement

Let us consider a quantum system $\mathcal{S}$ that is composed of two subsystems $\mathcal{S}_A$ and $\mathcal{S}_B$. The two subsystems $\mathcal{S}_A$ and $\mathcal{S}_B$ are said to be entangled with one another if the state of the system $\mathcal{S}$ *cannot* be written as a product of any two states of the individual subsystems. That is, the total state $|\Psi\rangle$ of the entire system $\mathcal{S}$ *cannot* be decomposed in the form

$$|\Psi\rangle = |\psi\rangle_A \otimes |\phi\rangle_B = |\psi\rangle_A |\phi\rangle_B \ . \tag{1.9}$$

for any two states $|\psi\rangle_A$ of $\mathcal{S}_A$ and $|\phi\rangle_B$ of $\mathcal{S}_B$. We shall now discuss the Bell states as a simple example of entangled states . If we consider a system of two spin-half particles A and B, described by their respective two-dimensional orthonormal bases $\{|\uparrow\rangle_i , |\downarrow\rangle_i\}$ where $i = A, B$, then the Bell states given by

$$|\Psi^{\pm}\rangle = \frac{1}{\sqrt{2}} \left(|\uparrow\rangle_A |\uparrow\rangle_B \pm |\downarrow\rangle_A |\downarrow\rangle_B \right) \tag{1.10}$$

$$|\Phi^{\pm}\rangle = \frac{1}{\sqrt{2}} \left(|\uparrow\rangle_A |\downarrow\rangle_B \pm |\downarrow\rangle_A |\uparrow\rangle_B \right) \ . \tag{1.11}$$

are entangled states and for any Bell state $|\Psi_i\rangle$ we claim that we cannot find any two states $|\psi\rangle_A$ and $|\phi\rangle_B$ such that

$$|\Psi_i\rangle = |\psi\rangle_A |\phi\rangle_B \ . \tag{1.12}$$

***Proof* :** Let us take, for example, the Bell state

$$|\Phi^{+}\rangle = \frac{1}{\sqrt{2}} \left(|\uparrow\rangle_A |\downarrow\rangle_B + |\downarrow\rangle_A |\uparrow\rangle_B \right) \ . \tag{1.13}$$

Let us say that there exist states $|\psi\rangle_A$ and $|\phi\rangle_B$ of the form

$$|\psi\rangle_A = a \,|\uparrow\rangle_A + b \,|\downarrow\rangle_A \text{ and} \tag{1.14}$$

$$|\phi\rangle_B = c \,|\uparrow\rangle_B + d \,|\downarrow\rangle_B \tag{1.15}$$

such that

$$\left|\Phi^+\right\rangle = |\psi\rangle_A \,|\phi\rangle_B \;. \tag{1.16}$$

Now,

$$|\psi\rangle_A \,|\phi\rangle_B = ac \,|\uparrow\rangle_A \,|\uparrow\rangle_B + ad \,|\uparrow\rangle_A \,|\downarrow\rangle_B + bc \,|\downarrow\rangle_A \,|\uparrow\rangle_B + bd \,|\downarrow\rangle_A \,|\downarrow\rangle_B \;. \tag{1.17}$$

Comparing this with Eq. (1.13), we find

$$ad = bc = \frac{1}{\sqrt{2}} \;, \tag{1.18}$$

$$ac = bd = 0 \;. \tag{1.19}$$

The equations in the first line of Eq. (1.19) imply that all the coefficients a, b, c, d have to be non-zero, whereas those in the second line imply otherwise . Hence the equations are inconsistent and the state $\left|\Phi^+\right\rangle$ is not separable, i.e. it is entangled . The same can be shown for the other three Bell states .

Let us pause for a moment to appreciate what the idea of entanglement physically corresponds to. It basically means that no individual quantum state can be ascribed to any two quantum subsystems that are entangled with one another and only a total state exists for the entire system . The idea of entanglement between the system and the environment and hence the loss of definite phase relations between the states of the system shall prove to be the key for explaining the evolution of open quantum systems from quantum behaviour to classical behaviour, as we shall see in the next chapter .

1.5 The density matrix formalism of quantum mechanics

We have seen in the previous section that if two systems are entangled with one another, individual quantum states cannot be ascribed to any of them. Hence, while studying the dynamics of such systems, the state vector formalism of quantum mechanics turns out to be insufficient. If we are performing measurements only on one of the systems, then the

statistics of that measurement cannot be represented by a state vector. It is in this context that the idea of density operators provides a much more elegant and efficient way of doing things. Given its relevance in studying open quantum systems, we shall briefly discuss the density operator formalism of quantum mechanics in this section.

1.5.1 Density matrices describing a pure state

If a system is known to be in a quantum state $|\Psi\rangle$, then it is said to be in a *pure state* and the density operator for the system $\hat{\rho}$ is given by

$$\hat{\rho} = |\Psi\rangle \langle\Psi| \ . \tag{1.20}$$

When this operator is represented in a particular basis, the resulting matrix is known as the density matrix. But the term 'density matrix' is used extensively in the literature for the density operator and we shall continue to use the two terms interchangeably.

Properties :

1. Trace of a pure state density matrix is equal to one .
   Proof : Let us expand $|\Psi\rangle$ in an orthonormal basis $\{|i\rangle\}$.

   $$|\Psi\rangle = \sum_i c_i |i\rangle \quad \text{where} \quad \sum_i c_i^* c_i = 1 \ . \tag{1.21}$$

   Now,

   $$\mathrm{Tr}(\hat{\rho}) = \sum_i \langle i|\hat{\rho}|i\rangle = \sum_i \langle i|\Psi\rangle \langle\Psi|i\rangle = \sum_i c_i c_i^* = 1 \ . \tag{1.22}$$

2. The expectation value of any observable $\hat{A}$ in a state with the density matrix $\hat{\rho}$ is given by $\mathrm{Tr}(\hat{\rho}\hat{A})$.
   Proof : Let us consider the eigenbasis $|a_i\rangle$ of the operator $\hat{A}$, i.e. $|a_i\rangle$ such that

   $$\hat{A}|a_i\rangle = a_i |a_i\rangle \ . \tag{1.23}$$

   Now,

   $$\mathrm{Tr}(\hat{\rho}\hat{A}) = \sum_i \langle a_i|\hat{\rho}\hat{A}|a_i\rangle = \sum_i \langle a_i|\Psi\rangle \langle\Psi|\hat{A}|a_i\rangle = \sum_i a_i \langle a_i|\Psi\rangle \langle\Psi|a_i\rangle$$

$$= \sum_i a_i |\langle a_i|\Psi\rangle|^2 = \langle\hat{A}\rangle_\Psi \equiv \langle\hat{A}\rangle_{\hat{\rho}} . \tag{1.24}$$

It might seem that this does not tell us everything about the statistics of measurements that we make with operator $\hat{A}$ on state $|\Psi\rangle$. It gives use the mean value of measurements. But, for example, what about the variance? While we cannot say anything about the variance using only $\text{Tr}(\hat{\rho}\hat{A})$, we just need to find $\text{Tr}(\hat{\rho}\hat{A}^2)$ and use the expression for variance as $\sigma_A^2 = \langle A^2\rangle - \langle A\rangle^2$. Likewise, expectation values of higher powers of the operator $\hat{A}$ can be found and the measurement statistics for any experiment can be evaluated.

3. The evolution of the pure-state density matrix $\hat{\rho}$ of a system with a Hamiltonian H is

$$i\hbar\frac{d\hat{\rho}}{dt} = [H, \hat{\rho}] . \tag{1.25}$$

Proof : The Schrödinger equation is given by

$$i\hbar\frac{d}{dt}|\Psi\rangle = H|\Psi\rangle . \tag{1.26}$$

Taking Hermitian conjugate of Eq. (1.26), we find

$$-i\hbar\frac{d}{dt}\langle\Psi| = \langle\Psi|H . \tag{1.27}$$

Now,

$$i\hbar\frac{d\hat{\rho}}{dt} = i\hbar\frac{d}{dt}(|\Psi\rangle\langle\Psi|) = i\hbar\left[|\Psi\rangle\frac{d}{dt}\langle\Psi| + \left(\frac{d}{dt}|\Psi\rangle\right)\langle\Psi|\right]$$
$$= \left(-|\Psi\rangle\langle\Psi|H + H|\Psi\rangle\langle\Psi|\right) = (H\hat{\rho} - \hat{\rho}H) = [H, \hat{\rho}] . \tag{1.28}$$

1.5.2 Density matrices describing a mixed state

Mixed-state density matrices represent systems whose quantum states are not entirely known. Let us say that the system is in one of the pure states $\{|\Psi_i\rangle\}$ with probabilities $\{p_i\}$, then the density matrix for the system is given by

$$\hat{\rho} = \sum_i p_i|\Psi_i\rangle\langle\Psi_i| = \sum_i p_i\hat{\rho}_i \quad \text{with} \quad \sum_i p_i = 1 , \tag{1.29}$$

where "$\hat{\rho}_i$"s are the ith pure-state density matrices. If one of the p_is is 1 and the rest are zero, we have the case of a pure-state density matrix. Otherwise, it is called a mixed-state density

matrix. Note that the states $\{|\Psi_i\rangle\}$, while normalized, are not assumed to be orthogonal to each other. (One could have a spin-$1/2$ system with 50% probability to be in state $|0\rangle$ and 50% probability to be in state $(1/\sqrt{2})\left[|0\rangle + |1\rangle\right]$.) We would like to point out here that Eq. (1.29) does not represent a system that is in a superposition of different pure quantum states. The system represented by Eq. (1.29) is actually in one of the pure states $\hat{\rho}_i$, its just that we do not know which pure state it is in. The mixed-state density matrix is just a tool that takes into account our ignorance about the actual state of the system and produces the correct measurement statistics (the correct expectation values for all operators) for such systems.

Up to now, we have emphasized the point that given an ensemble $\{p_i,\ |\Psi_i\rangle\}$, we can construct the mixed density matrix for the system and be sure that the system is actually in any one of the states $\{|\Psi_i\rangle\}$. But the converse is not true. For example, if we are given a mixed density matrix and are asked which particular ensemble it corresponds to, there is no unique answer. In fact, one can prove that two ensembles $\{p_i,\ |\Psi_i\rangle\}$ and $\{q_j,\ |\Phi_j\rangle\}$ will correspond to the same density matrix if [9]

$$\sqrt{p_i}\,|\Psi_i\rangle = \sum_j U_{ij}\sqrt{q_j}\,|\Phi_j\rangle\ , \tag{1.30}$$

where U_{ij} are elements of a unitary matrix. This works even if the two ensembles are not of the same size since we can add states with zero probabilities in the smaller ensemble to make sizes of both the ensembles equal.

Proof :

$$\hat{\rho} = \sum_i p_i |\Psi_i\rangle\langle\Psi_i| = \sum_i \sqrt{p_i}|\Psi_i\rangle\langle\Psi_i|\sqrt{p_i^*} = \sum_i \left(\sum_j U_{ij}\sqrt{q_j}\,|\Phi_j\rangle \sum_k U_{ik}^*\sqrt{q_k^*}\,\langle\Phi_k| \right)$$

$$= \sum_{jk} \left(\sqrt{q_j q_k}\,|\Phi_j\rangle\langle\Phi_k| \sum_i U_{ij}U_{ik}^* \right) = \sum_{jk} \left[\sqrt{q_j q_k}\,|\Phi_j\rangle\langle\Phi_k| \sum_i \left(U^\dagger U\right)_{kj} \right]$$

$$= \sum_{jk} \sqrt{q_j q_k}\,|\Phi_j\rangle\langle\Phi_k|\ \delta_{kj} = \sum_j q_j\,|\Phi_j\rangle\langle\Phi_j|\ . \tag{1.31}$$

All the properties that we proved for pure state density matrices hold true for mixed-state density matrices as well. For the sake of completeness, we shall briefly discuss some proofs here.

1. Trace of a mixed-state density matrix is unity.

Proof :

$$
\begin{aligned}
\mathrm{Tr}(\hat{\rho}) &= \mathrm{Tr}\Big(\sum_i p_i \hat{\rho}_i\Big) \\
&= \sum_i p_i \mathrm{Tr}(\hat{\rho}_i) \\
&= \sum_i p_i \qquad (\text{as } \mathrm{Tr}(\hat{\rho}_i) = 1) \\
&= 1 \qquad \Big(\text{as } \sum_i p_i = 1\Big) .
\end{aligned}
\tag{1.32}
$$

Here we have used Eq. (1.22).

2. The expectation value of any observable $\hat{A}$ for a system with a mixed-state density matrix $\hat{\rho}$ is just the sum of the expectation values of $\hat{A}$ in the ith state weighted by the respective probabilities p_i. This is given by $\mathrm{Tr}(\hat{\rho}\hat{A})$.

   Proof :

$$
\begin{aligned}
\mathrm{Tr}(\hat{\rho}\hat{A}) &= \sum_i p_i \mathrm{Tr}(\hat{\rho}_i \hat{A}) \\
&= \sum_i p_i \langle \hat{A} \rangle_{\hat{\rho}_i} \\
&= \langle \hat{A} \rangle_{\hat{\rho}} ,
\end{aligned}
\tag{1.33}
$$

   where we have used Eq. (1.24).

3. The evolution of the mixed-state density matrix $\hat{\rho}$ of a system with a Hamiltonian H is given by

$$
i\hbar \frac{d\hat{\rho}}{dt} = [H, \hat{\rho}] .
\tag{1.34}
$$

   Proof :

$$
\begin{aligned}
i\hbar \frac{d\hat{\rho}}{dt} &= \sum_i p_i \Big(i\hbar \frac{d\hat{\rho}_i}{dt} \Big) \\
&= \sum_i p_i [H, \hat{\rho}_i] \\
&= [H, \sum_i p_i \hat{\rho}_i] \\
&= [H, \hat{\rho}] ,
\end{aligned}
\tag{1.35}
$$

   using Eq. (1.28)

1.5.3 Entropy of a mixed state

For a system that is in a mixed state, we do not know for certain which pure state the system is in. But the degree of ignorance about the actual state of the system will vary from one mixed state to another. For example, if a system is in either one of the states $|\Psi_1\rangle$ and $|\Psi_2\rangle$ with equal probabilities, then the amount of ignorance about the state of the system is higher than if, say, the system is in state $|\Psi_1\rangle$ with 90% probability and $|\Psi_2\rangle$ with 10% probability. Hence, to quantify the degree of mixedness of a state, we shall introduce the notion of entropy of a density matrix. Let us first see how can we distinguish a pure-state density matrix from a mixed-state one.

Distinguishing pure-state and mixed-state density matrices:

For a pure-state density matrix,

$$\hat{\rho}^2 = \hat{\rho} \Rightarrow \text{Tr}(\hat{\rho}^2) = 1 \ , \tag{1.36}$$

but this does not hold true for mixed state density matrices.

Proof: For a pure state density matrix, we have

$$\hat{\rho^2}_{pure} = |\Psi\rangle\langle\Psi|\Psi\rangle\langle\Psi| = |\Psi\rangle\langle\Psi| = \hat{\rho}_{pure} \ , \tag{1.37}$$

whereas for a mixed state density matrix from Eq. (1.29),

$$\hat{\rho^2}_{mixed} = \sum_{i,j} p_i p_j |\Psi_i\rangle\langle\Psi_i|\Psi_j\rangle\langle\Psi_j| \ . \tag{1.38}$$

For Eq. (1.38) to be equal to $\hat{\rho}_{mixed}$, we need

$$p_i p_j \left\langle \Psi_i \big| \Psi_j \right\rangle = p_i \delta_{ij} \ . \tag{1.39}$$

This would first of all require the states $\{|\Psi_i\rangle\}$ to be orthogonal, which, as we have noted before, need not be the case for a general mixed state density matrix. Even if they were orthogonal, we would need $p_i^2 = p_i$, which is only possible if one of the p_is is 1 and the rest are 0 (since they have to sum to 1)—the case of a pure-state density matrix. For a mixed-state density matrix, Eq. (1.39) can never be satisfied. For such a system, $\text{Tr}(\hat{\rho}^2) < 1$.

Von Neumann entropy

The von Neumann entropy of a state $\hat{\rho}$ is given by[9]

$$S = -\operatorname{Tr}(\hat{\rho} \log_2 \hat{\rho}) . \tag{1.40}$$

Let us work in the eigenbasis of the density matrix, i.e., $\hat{\rho} = \sum_i a_i |i\rangle\langle i|$. Now,

$$
\begin{aligned}
\operatorname{Tr}(\hat{\rho} \log_2 \hat{\rho}) &= \sum_i \langle i|\hat{\rho} \log_2 \hat{\rho}|i\rangle \\
&= \sum_{ijk} a_j \langle i|j\rangle\langle j|\log_2 a_k |k\rangle\langle k|i\rangle \\
&= \sum_{ijk} a_j \delta_{ij} \log_2(a_k) \langle j|k\rangle \langle k|i\rangle \\
&= \sum_{ijk} a_j \delta_{ij} \log_2(a_k) \delta_{jk} \delta_{ki} \\
&= \sum_i a_i \log_2 a_i .
\end{aligned}
\tag{1.41}
$$

In the case when one of the eigen values is zero, we take its contribution $0 \log_2 0$ to be 0. This is physically justified since we are just stating that a state that is not present will not make a contribution to the entropy. Since a_is are probablilites that lie between 0 and 1, the von Neumann entropy is never negative. For a pure state, one of the eigenvalues is 1 and the rest are zero. Hence the von Neumann entropy attains its minimum value, zero, at pure states. The maximum will obviously occur when all the eigen values have the same value. For an $N \times N$ density matrix, the von Neumann entropy will then be given by

$$S = -\sum_{i=1}^{N} \frac{1}{N} \log_2 \frac{1}{N} = -N \times \frac{1}{N}(-\log_2 N) = \log_2 N . \tag{1.42}$$

The density matrix for such a case is given by

$$\hat{\rho} = \sum_{i=1}^{N} \frac{1}{N} |\Psi_i\rangle\langle\Psi_i| , \tag{1.43}$$

and the state of the system is called *maximally mixed*. Since $\hat{\rho}$ is a Hermitian matrix, the eigen vectors corresponding to *distinct* eigen values are orthogonal. Even though here the eigen values are not distinct, one can use the fact that any linear combination of eigen vectors is again an eigen vector and perform a Gram-Schmidt orthogonalization to obtain an

orthonormal basis of eigen vectors. Thus, such a density matrix can be obtained, for example, by creating a mixture of N orthogonal, and thus mutually exclusive, states with equal probability.

Hence, the von Neumann entropy can take a minimum value of zero for pure states, while its maximum value, in the space of N pure states, is $\log_2 N$ for maximally mixed states.

1.5.4 Reduced density matrices

We have already seen in Section 1.4 that for two quantum systems A and B that are entangled with one another, no individual quantum state can be ascribed to either of them. But if we have an observer who has access to system A alone and is performing local measurements on system A, there is a tool that can essentially produce all the local measurement statistics. This is known as the reduced density matrix of the system. We shall define this object and discuss some of its properties here.

Let us say we have two systems A and B which are entangled with one another and the state of the combined system AB is given by $\hat{\rho}$, then the reduced density matrices for the systems A and B are defined by

$$\hat{\rho}_A = \mathrm{Tr}_B\big(\hat{\rho}\big) \quad \text{and} \quad \hat{\rho}_B = \mathrm{Tr}_A\big(\hat{\rho}\big) . \tag{1.44}$$

Here Tr_B is known as the partial trace over system B. Let us formally define what that means. If $\{\Psi_k\}$ and $\{\Phi_l\}$ are the orthonormal basis of systems A and B respectively and $\hat{O}_A$ and $\hat{O}_B$ are operators on respective systems, then

$$\mathrm{Tr}_B\big(\hat{O}_A \otimes \hat{O}_B\big) = \hat{O}_A \mathrm{Tr}_B\big(\hat{O}_B\big) = \hat{O}_A \sum_l \langle \Phi_l|\hat{O}_B|\Phi_l\rangle . \tag{1.45}$$

We shall now give a concrete example of the reduced density matrix of a system. Let us take the Bell state

$$\big|\Psi^+\big\rangle = \frac{1}{\sqrt{2}}\big[\, |0_A\rangle\,|0_B\rangle + |1_A\rangle\,|1_B\rangle \,\big] = \frac{1}{\sqrt{2}}\sum_{i=0}^{1} |i_A\rangle\,|i_B\rangle , \tag{1.46}$$

where $|0_i\rangle, |1_i\rangle$ respectively represent the spin-up and spin-down states of two spin-half particles A and B. Now the reduced density matrix for the system A is given by

$$\hat{\rho}_A = \frac{1}{2}\mathrm{Tr}_B\Big(\sum_{i,j=0}^{1} |i_A\rangle\,|i_B\rangle\,\langle j_A|\,\langle j_B| \Big)$$

$$
\begin{aligned}
&= \frac{1}{2} \sum_{ijk=0}^{1} |i_A\rangle\langle j_A| \, \langle k_B|i_B\rangle \, \langle j_B|k_B\rangle \\
&= \frac{1}{2} \sum_{ijk=0}^{1} |i_A\rangle\langle j_A| \delta_{ki}\delta_{jk} \\
&= \frac{1}{2} \sum_{i=0}^{1} |i_A\rangle\langle i_A| \\
&= \frac{|0_A\rangle\langle 0_A| + |1_A\rangle\langle 1_A|}{2} \\
&= \frac{I_A}{2} \, .
\end{aligned}
\tag{1.47}
$$

Note that $\hat{\rho}_A$ is a mixed state since $\mathrm{Tr}(\hat{\rho}_A^2) = \frac{1}{4}\mathrm{Tr}(I_A) = \frac{1}{2}$ which is less than 1. So we can clearly see here that although the total state of AB is known, the reduced density matrix of system A is a mixed state, implying that we do not exactly know which state it is in. Note that the same density matrix can also be obtained by preparing the system A by a random process to have 50% probability of being in a pure state $|0_A\rangle$ and 50% probability of being in a pure state $|1_A\rangle$. But here there is no notion of A existing in a pure state. It is just that it is part of a larger system AB and the measurement statistics are represented by the above reduced density matrix when we have access only to A. But, as we have seen, the two scenarios are same at the level of density matrices and, hence, measurement statistics.

We shall end the discussion of density matrices by showing that the reduced density matrices indeed provide the correct measurement statistics for local measurements. Let us say $\{\Psi_k\}$ and $\{\Phi_l\}$ are the orthonormal basis of systems A and B respectively and consider an operator $\hat{O}$ which acts on system A alone. These are represented by $\hat{O} = \hat{O}_A \otimes \hat{I}_B$ where $\hat{I}_B$ is the identity operator on the Hilbert space of B. Now the expectation value for the combined state $\hat{\rho}$ of such an observable $\hat{O}_A$ is given by [11]

$$
\begin{aligned}
\langle\hat{O}\rangle &= \mathrm{Tr}(\hat{\rho}\hat{O}) \\
&= \sum_{kl} \langle\Phi_l| \, \langle\Psi_k| \, \hat{\rho}(\hat{O}_A \otimes \hat{I}_B) \, |\Psi_k\rangle \, |\Phi_l\rangle \\
&= \sum_{k} \langle\Psi_k| \left(\sum_{l} \langle\Phi_l|\hat{\rho}|\Phi_l\rangle \right) \hat{O}_A \, |\Psi_k\rangle \\
&= \sum_{k} \langle\Psi_k| \, (\mathrm{Tr}_B\hat{\rho})\hat{O}_A \, |\Psi_k\rangle \\
&= \sum_{k} \langle\Psi_k| \, \hat{\rho}_A\hat{O}_A \, |\Psi_k\rangle
\end{aligned}
$$

$$= \text{Tr}_A(\hat{\rho}_A \hat{O}_A) \ . \tag{1.48}$$

This shows that the reduced density matrices produce correct local measurement statistics.

1.6 Wigner functions

1.6.1 Introduction: The necessity of Wigner functions

In quantum mechanics, given the wave function $\psi(x)$ of a system, the probability density in position space is given by $|\psi(x)|^2$. But if we want to find the momentum space probability density $\phi(p)$, we need to perform the integral

$$\phi(p) = \frac{1}{\sqrt{2\pi\hbar}} \int \psi(x) e^{-\frac{ipx}{\hbar}} \, dx \ . \tag{1.49}$$

Even if the integral is not difficult to perform, it is a bit difficult to visualize the momentum space density distribution if one is given $\psi(x)$ alone. Also, classical mechanics, explored in the phase space of coordinates and momenta, provides us with insights not obtained from a study in coordinate space, even if the results from both approaches are equivalent.

It is thus desirable to have a function that incorporates information about both the position space and momentum space probability densities and such a function would naturally be defined on phase space. The Wigner function was built for just that purpose, as a probability density on phase space. But one needs to take into account, in the context of quantum mechanics, the uncertainty principle which forbids the simultaneous precise measurement of observables that do not commute with one another. This essentially imposes certain conditions on the Wigner function. The direct consequence one can perceive is that the Wigner function cannot be localised beyond a limit imposed by the uncertainty principle. If one attempts to localize it too much in the x-direction, one would necessarily have to allow for an increase in spread in the momentum direction. Another property that sets the Wigner function apart from a usual probability distribution is that the Wigner function can turn negative. Thus, instead of a probability distribution function in phase space, we get what is called a quasi-probability distribution.

As we have stated before, classical systems are best described by trajectories in phase space. But quantum systems are described by abstract vectors in Hilbert space. Thus, it is

useful to have a phase space description of quantum mechanics for the study of the correspondence between classical and quantum mechanics and the quantum-to-classical transition. This is our main point of interest in Wigner functions.

We shall provide a brief description of Wigner functions in this section.

1.6.2 Definition

Let us consider a state $|\Psi\rangle$ whose position space representation is given by $\Psi(x,t)$ and momentum space wave function is given by $\Phi(p,t)$. The Wigner function of such a state is defined to be

$$
\begin{aligned}
W(x,p,t) &= \frac{1}{\pi\hbar} \int_{-\infty}^{\infty} dy\, \Psi(x-y,t)\Psi^*(x+y,t)e^{\frac{2ipy}{\hbar}} \\
&= \frac{1}{\pi\hbar} \int_{-\infty}^{\infty} dy\, \langle x-y|\Psi\rangle\langle\Psi|x+y\rangle e^{\frac{2ipy}{\hbar}} \\
&= \frac{1}{\pi\hbar} \int_{-\infty}^{\infty} dy\,dp'\,dp'' \langle x-y|p'\rangle\langle p'|\Psi\rangle\langle\Psi|p''\rangle\langle p''|x+y\rangle e^{\frac{2ipy}{\hbar}} \\
&= \frac{1}{\pi\hbar} \int_{-\infty}^{\infty} dy\,dp'\,dp'' \Big(\frac{1}{\sqrt{2\pi\hbar}}e^{\frac{ip'(x-y)}{\hbar}}\Big)\Phi(p',t)\Phi^*(p'',t)\Big(\frac{1}{\sqrt{2\pi\hbar}}e^{-\frac{ip''(x+y)}{\hbar}}\Big)e^{\frac{2ipy}{\hbar}} \\
&= \frac{1}{\pi\hbar(2\pi\hbar)} \int_{-\infty}^{\infty} dp'\,dp''\,dy\, e^{\frac{i(2p-p'-p'')y}{\hbar}}\Phi(p',t)\Phi^*(p'',t)e^{\frac{i(p'-p'')x}{\hbar}} \\
&= \frac{1}{\pi\hbar} \int_{-\infty}^{\infty} dp'\,dp''\,\delta(2p-p'-p'')\Phi(p',t)\Phi^*(p'',t)e^{\frac{i(p'-p'')x}{\hbar}} \\
&= \frac{1}{\pi\hbar} \int_{-\infty}^{\infty} dp''\,\Phi(2p-p'',t)\Phi^*(p'',t)e^{\frac{2i(p-p'')x}{\hbar}} \\
&= \frac{1}{\pi\hbar} \int_{-\infty}^{\infty} dq\,\Phi(p-q,t)\Phi^*(p+q,t)e^{\frac{-2iqx}{\hbar}}
\end{aligned}
\tag{1.50}
$$
$$
\text{where} \quad p'' = p+q \,.
$$

It can also be written as

$$
W(x,p,t) = \frac{1}{\pi\hbar} \int dy\, \langle x-y|\hat{\rho}|x+y\rangle e^{\frac{2ipy}{\hbar}} \tag{1.51}
$$

$$
= \frac{1}{\pi\hbar} \int dq\, \langle p-q|\hat{\rho}|p+q\rangle e^{-\frac{2ixq}{\hbar}} \tag{1.52}
$$

which can be generalized to mixed state density matrices as well.

1.6.3 Properties

1. The Wigner function of any quantum system is always real.

   Proof :

   $$W(x,p,t) = \frac{1}{\pi\hbar} \int_{-\infty}^{\infty} dy \Psi(x-y,t)\Psi^*(x+y,t) e^{\frac{2ipy}{\hbar}}$$

   $$\Rightarrow W^*(x,p,t) = \frac{1}{\pi\hbar} \int_{-\infty}^{\infty} dy \Psi^*(x-y,t)\Psi(x+y,t) e^{\frac{-2ipy}{\hbar}}$$

   $$= -\frac{1}{\pi\hbar} \int_{\infty}^{-\infty} dy' \Psi^*(x+y',t)\Psi(x-y',t) e^{\frac{2ipy'}{\hbar}} \quad \text{with} \quad y' = -y$$

   $$= \frac{1}{\pi\hbar} \int_{-\infty}^{\infty} dy' \Psi(x-y',t)\Psi^*(x+y',t) e^{\frac{2ipy'}{\hbar}}$$

   $$= W(x,p,t) \ . \tag{1.53}$$

2. The position and momentum space probability densities are given by

   $$|\Psi(x,t)|^2 = \int_{-\infty}^{\infty} dp\, W(x,p,t) \quad \text{and} \quad |\Phi(p,t)|^2 = \int_{-\infty}^{\infty} dx\, W(x,p,t) \ . \tag{1.54}$$

   Proof :

   $$\int_{-\infty}^{\infty} dp\, W(x,p,t) = \frac{1}{\pi\hbar} \int_{-\infty}^{\infty} dp\,dy \Psi(x-y,t)\Psi^*(x+y,t) e^{\frac{2ipy}{\hbar}}$$

   $$= \int_{-\infty}^{\infty} dy \delta(y)\Psi(x-y,t)\Psi^*(x+y,t)$$

   $$= \Psi(x,t)\Psi^*(x,t)$$

   $$= |\Psi(x,t)|^2 \ , \tag{1.55}$$

   where we have used

   $$\frac{1}{\pi\hbar} \int_{-\infty}^{\infty} dp\, e^{\frac{2ipy}{\hbar}} = \delta(y) \ . \tag{1.56}$$

   A similar proof can be given for the momentum space probability density.

3. The integral of the Wigner function over the entire phase space is unity.

   Proof :

   $$\int_{-\infty}^{\infty} dp\, dx\, W(x,p,t) = \int_{-\infty}^{\infty} dx\, |\Psi(x,t)|^2 = 1 \ , \tag{1.57}$$

   using Eq. (1.54).

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4. Expectation values of observables are found by averaging them over the entire phase space. That is[1]

$$\langle \hat{O} \rangle = \int dx dp W(x,p)\tilde{O}(x,p) \, , \tag{1.58}$$

where $\tilde{O}(x,p)$ is known as the Weyl transform of the operator $\hat{O}$, defined by

$$\tilde{O}(x,p) = 2\int dy \langle x+y|\hat{O}|x-y\rangle e^{-\frac{2ipy}{\hbar}}$$

$$= 2\int du \langle p+u|\hat{O}|p-u\rangle e^{\frac{2ixu}{\hbar}} \, . \tag{1.59}$$

$$\tag{1.60}$$

Proof:

$$\langle \hat{O} \rangle = Tr(\hat{\rho}\hat{O}) = \int dx' dp' \langle x'|\hat{\rho}|p'\rangle \langle p'|\hat{O}|x'\rangle$$

$$= \int dx' dx'' dp' dp'' \langle x'|\hat{\rho}|x''\rangle \langle x''|p'\rangle \langle p'|\hat{O}|p''\rangle \langle p''|x'\rangle \, . \tag{1.61}$$

Now we let $x' = x - y$, $x'' = x + y$ and $p' = p + u$, $p'' = p - u$. Also using

$$\langle x|p \rangle = \frac{1}{\sqrt{2\pi\hbar}}\exp\left\{\frac{ipx}{\hbar}\right\} \, , \quad dx' dx'' = 2dx dy \quad \text{and} \quad dp' dp'' = 2dp du \tag{1.62}$$

in Eq. (1.61) yields

$$\langle \hat{O} \rangle = \frac{4}{2\pi\hbar}\int dx dy dp du \langle x-y|\hat{\rho}|x+y\rangle e^{\frac{i(p+u)(x+y)}{\hbar}} \langle p+u|\hat{O}|p-u\rangle e^{-\frac{i(p-u)(x-y)}{\hbar}}$$

$$= \int dx dp \left[\frac{1}{\pi\hbar}\int dy \langle x-y|\hat{\rho}|x+y\rangle e^{\frac{2ipy}{\hbar}}\right]\left[2\int du \langle p+u|\hat{O}|p-u\rangle e^{\frac{2ixu}{\hbar}}\right]$$

$$= \int dx dp W(x,p)\tilde{O}(x,p) \, . \quad \text{[Q.E.D]} \tag{1.63}$$

Although we can see that the Wigner function encodes information about both the position and momentum space probability density, we should keep in mind that it is not a model probability distribution function because of its negative tendencies, i.e., for some states, it can take negative values in some regions of phase space.

1.6.4 Examples of Wigner functions for various quantum systems

Having discussed the utility of Wigner functions and some of its prime properties, we would now illustrate the behavior of the Wigner functions of various quantum systems to understand how it looks and the ways in which it differs from a classical probability distribution.

Wigner function for a coherent state :   Let us consider a quantum harmonic oscillator having Hamiltonian of the form

$$\hat{H} = \frac{\hat{p}^2}{2m} + \frac{1}{2}m\omega^2\hat{x}^2 \ , \tag{1.64}$$

where symbols bear their usual meaning.

Coherent states $\{|\alpha\rangle\}$ are minimum uncertainty states of the harmonic oscillator potential and are the eigenstates of the annihilation operator with an eigenvalue α. They are given by

$$\hat{a}\,|\alpha\rangle = \alpha\,|\alpha\rangle \ , \tag{1.65}$$

where we have defined the creation operator ($\hat{a}^\dagger$) and the annihilation operator ($\hat{a}$) by the following expressions:

$$\hat{a} = \sqrt{\frac{m\omega}{2\hbar}}\hat{x} + i\frac{1}{\sqrt{2\hbar m\omega}}\hat{p} \quad , \quad \hat{a}^\dagger = \sqrt{\frac{m\omega}{2\hbar}}\hat{x} - i\frac{1}{\sqrt{2\hbar m\omega}}\hat{p} \ . \tag{1.66}$$

The expectation values of position and momentum for a coherent state $|\alpha\rangle$ can be found to be

$$\langle\hat{x}\rangle_\alpha = \langle\alpha|\hat{x}|\alpha\rangle = Re(\alpha)\sqrt{\frac{2\hbar}{m\omega}} \quad \text{and} \quad \langle\hat{p}\rangle_\alpha = \langle\alpha|\hat{p}|\alpha\rangle = Im(\alpha)\sqrt{2\hbar m\omega} \ . \tag{1.67}$$

Hence, we can say that the eigenvalue of a coherent state $|\alpha\rangle$ is

$$\alpha = \sqrt{\frac{m\omega}{2\hbar}}\,\langle\hat{x}\rangle_\alpha + i\frac{1}{\sqrt{2\hbar m\omega}}\,\langle\hat{p}\rangle_\alpha \ . \tag{1.68}$$

Now let us find the position space representation of coherent states ($\Psi_\alpha(x)$), which can be easily done by solving the differential equation obtained by writing Eq. (1.65) in position representation:

$$\sqrt{\frac{\hbar}{2m\omega}}\frac{d\Psi_\alpha(x)}{dx} + \sqrt{\frac{m\omega}{2\hbar}}\,x\Psi_\alpha(x) = \alpha\Psi_\alpha(x) \ . \tag{1.69}$$

Eq. (1.69) is solved by

$$\Psi_\alpha(x) = c\exp\left\{-\frac{m\omega}{2\hbar}x^2 + \sqrt{\frac{2m\omega}{\hbar}}\alpha x\right\} \ . \tag{1.70}$$

The constant can be fixed by normalization. Denoting by x_0 and p_0 the respective expectation values of position and momentum of the coherent state $|\alpha\rangle$, we have

$$\alpha = \sqrt{\frac{m\omega}{2\hbar}}x_0 + i\frac{1}{\sqrt{2\hbar m\omega}}p_0 \ , \tag{1.71}$$

and the normalized solution is

$$\Psi_\alpha(x) = \left(\frac{m\omega}{\pi\hbar}\right)^{\frac{1}{4}} \exp\left\{\frac{ip_0 x}{\hbar} - \frac{m\omega}{2\hbar}(x - x_0)^2\right\} . \tag{1.72}$$

One of the prime features of a coherent state is that is that if we let it evolve in time, it still remains a coherent state. At time t, the state given by Eq. (1.72) becomes

$$\Psi_\alpha(x, t) = \left(\frac{m\omega}{\pi\hbar}\right)^{\frac{1}{4}} \exp\left\{\frac{ip_t x}{\hbar} - \frac{m\omega}{2\hbar}(x - x_t)^2\right\} , \tag{1.73}$$

where

$$x_t = x_0 \cos(\omega t) + \frac{p_0}{m\omega} \sin\omega t , \tag{1.74a}$$

$$p_t = p_0 \cos\omega t - m\omega x_0 \sin\omega t . \tag{1.74b}$$

Note that Eq. (1.74) describes the classical phase space trajectory of a particle that starts out in harmonic oscillator potential with initial position and momentum x_0 and p_0, respectively.

With the wave function at our hand, we are in a position to find the Wigner function of a coherent state and study its behavior. The Wigner function for the state $\Psi_\alpha(x, t)$ turns out to be

$$W(x, p, t) = \frac{1}{\pi\hbar} \exp\left\{-\frac{m\omega}{\hbar}(x - x_t)^2 - \frac{1}{m\omega\hbar}(p - p_t)^2\right\} . \tag{1.75}$$

Note that the Gaussian is peaked at x_t, p_t which is the classical solution for the system. The evolution of this Wigner function is shown in Fig. 1.3.

A few features of the Wigner function are quite noteworthy. We can explicitly see that the peak of the Gaussian traces out the trajectory of the classical solution of the system. Moreover the spread of the Gaussian is a measure of the uncertainty of the state and the fact that the spread of the Gaussian remains constant as it circles around the phase space, implies that it remains a minimum uncertainty state throughout its evolution.

Wigner function for a Gaussian wave packet following free particle trajectory: Now we shall discuss the example of the Wigner function of a Gaussian wave packet evolving under no force and hence following a free particle trajectory. The normalized, time-dependent wave function that we shall consider is[1]

$$\Psi(x, t) = \left(\sqrt{\pi}\alpha F(t)\hbar\right)^{-\frac{1}{2}} \exp\left\{\frac{i[p_0(x - x_0) - \frac{p_0^2 t}{2m}]}{\hbar}\right\} \exp\left\{-\frac{[x - x_0 - \frac{p_0 t}{m}]^2}{2\alpha^2\hbar^2 F(t)}\right\} , \tag{1.76}$$

---

[1] For a derivation of this and related properties, see Nicholas Wheeler's essay titled "Gaussian Wavepackets" here.

(a) time = 0

(b) time = $\pi/2$

(c) time = π

(d) time = $2\pi/3$

(e) time = 2π

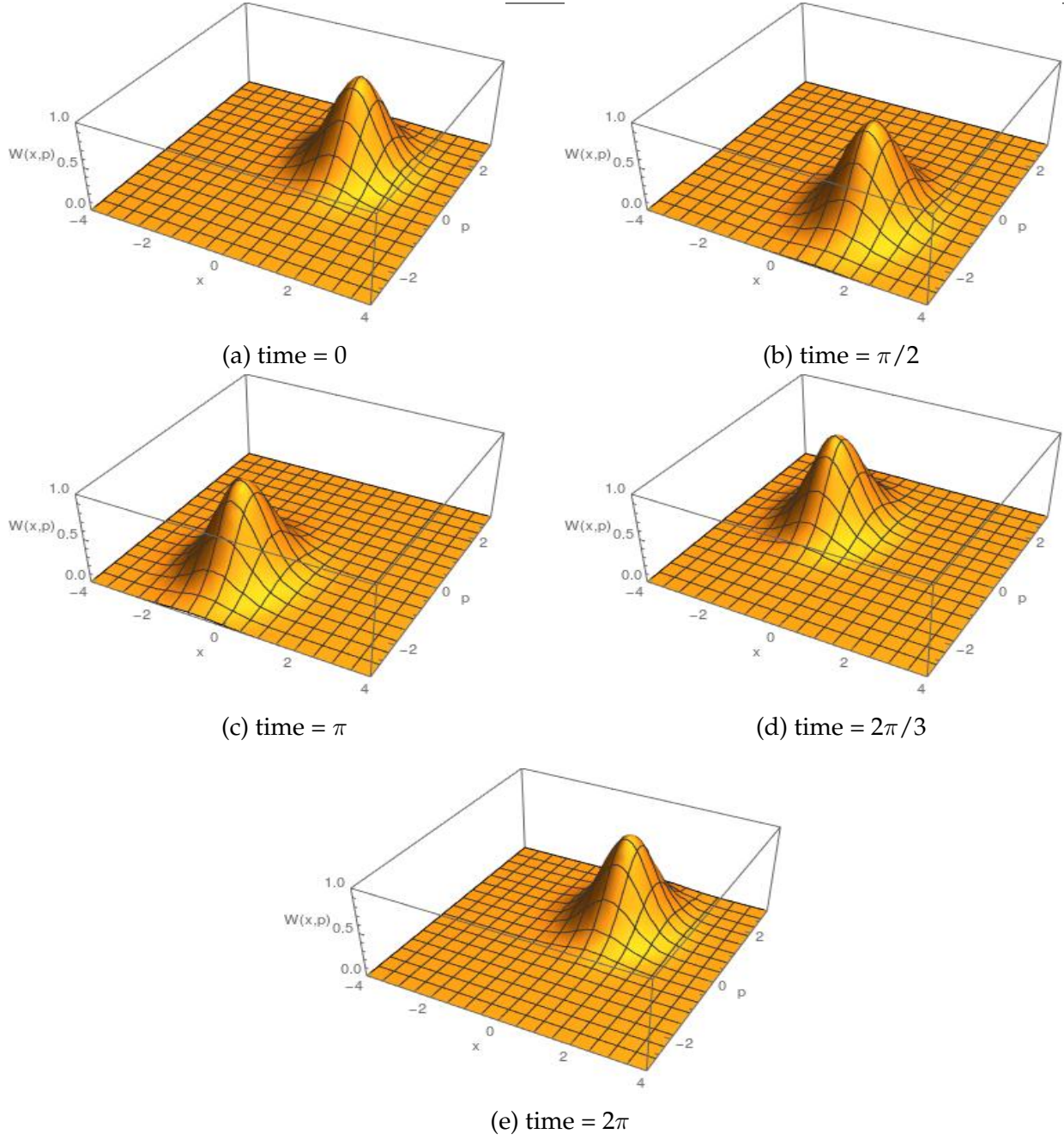Figure 1.3: Time evolution of the Wigner function associated with the coherent state given by Eq. (1.73). The parameters have been chosen to be $m = \omega = \hbar = x_0 = p_0 = 1$. Note that the Gaussian has its initial peak at (1,1) and it circles around the phase-space just like the classical solution.

where $F(t)$ is defined to be

$$F(t) = 1 + i(t/\tau) \quad \text{with} \quad \tau = m\hbar\alpha^2 \tag{1.77}$$

and α is a constant that characterizes the initial width of the Gaussian. The peak of the wave function is always situated at $x = x_0 + p_0 t/m$, which is precisely the classical trajectory of a free particle whose initial position and momentum are x_0 and p_0 respectively.

The integral which we need to perform to find the Wigner function for the state given by Eq. (1.76) is a bit lengthy. Here we quote only the end result:

$$W(x, p, t) = \frac{1}{\pi\hbar} \exp\left\{ -\frac{(x - x_0 - p_0 t/m)^2 + [(x - x_0 - p_0 t/m)\frac{t}{\tau} - \alpha^2\hbar(p - p_0)(1 + t^2/\tau^2)]^2}{\alpha^2\hbar^2(1 + \frac{t^2}{\tau^2})} \right\}.$$

(1.78)

(a) time = 0

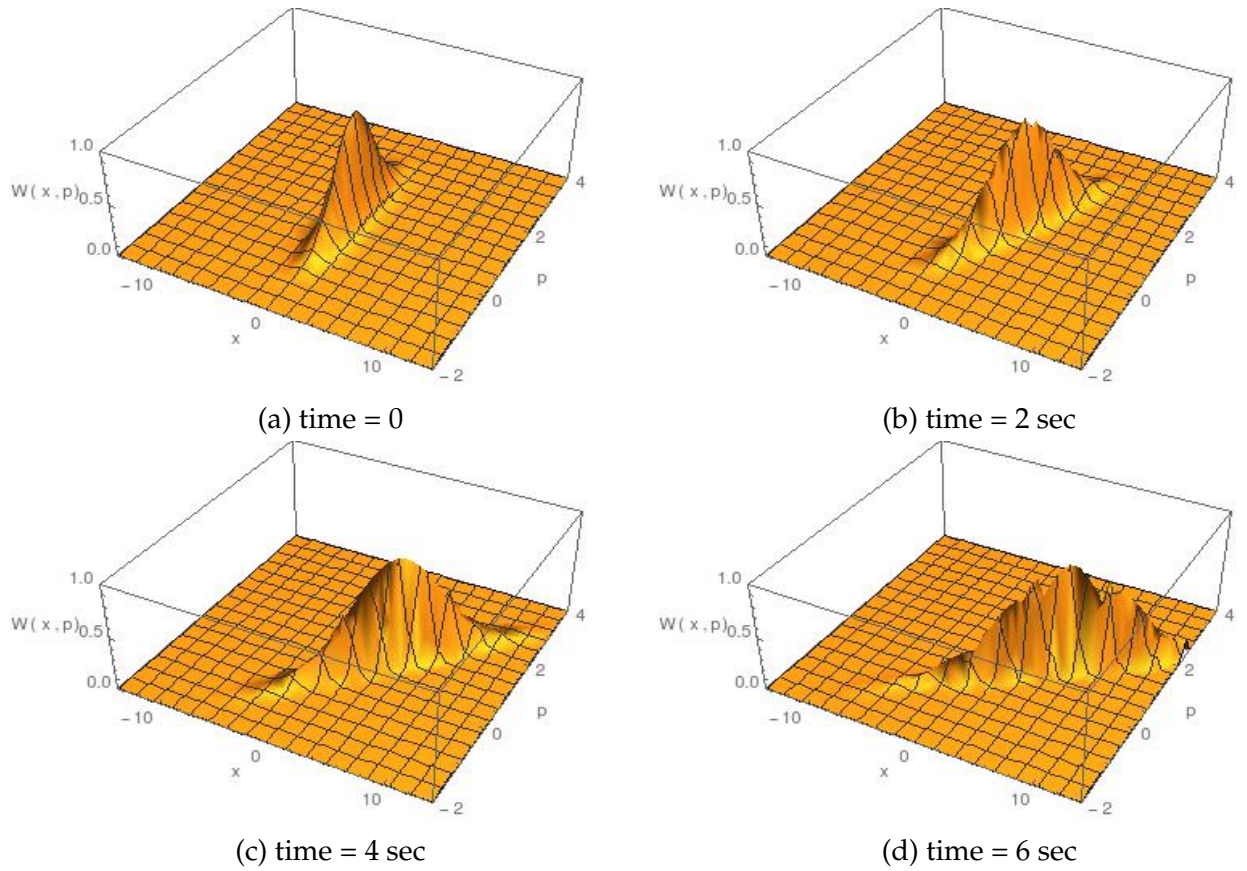(b) time = 2 sec

(c) time = 4 sec

(d) time = 6 sec

Figure 1.4: Time evolution of the Wigner function (Eq. (1.78)) associated with the Gaussian wavefunction following a free particle trajectory, described by Eq. (1.76). The initial position has been taken to be zero ($x_0 = 0$) and the initial momentum has been set to one ($p_0 = 1$). Also all the other parameters have been set to unity, i.e., $m = \alpha = \hbar = 1$. Notice that the momentum coordinate of the peak remains at 1 and its position coordinate is increasing linearly with time, just like a classical particle with similar initial conditions.

The Wigner function given by Eq. (1.78) has been plotted in Fig. 1.4. We can observe here

as well that the peak of the Gaussian follows the classical trajectory. One of the aspects in which the evolution of this Wigner function differs from that of a coherent state is in terms of its spread. We can notice that the spread of the Wigner function increases with time, implying an increase in the uncertainty associated with the state. This is also borne out by algebraic calculation.

Now we are in possession of the various tools which are needed to study decoherence and we shall begin the discussion of decoherence in the next chapter.

Chapter 2

Decoherence: an introduction

2.1 Introduction

Before we begin our discussion of decoherence, we must first understand what we mean by coherence. In a very crude manner, quantum coherence can be said to be a measure of the quantumness of a state. We have already shown in the previous chapter that a superposition of definite states is also a valid state in quantum mechanics and the superposition can manifest itself in the form of interference effects in suitable measurements. Decoherence can be said to be the loss of definite phase relations between the different components of a superposition state. Usually it is caused by the interaction of the environment with the system. But the effect of environmental interaction is very different in classical and quantum mechanics. In classical mechanics, the environment can effect the dynamics of the system by changing its momentum. If the environmental perturbation is weak in terms of the momentum carried by it, then its existence can essentially be entirely ignored. But the situation is quite different in its

Figure 2.1: Classical and quantum scattering. [Figure taken from [11]]

quantum counterpart. In the quantum picture what is more important is that the interaction entangles the environment with the system and it transports coherence from the local
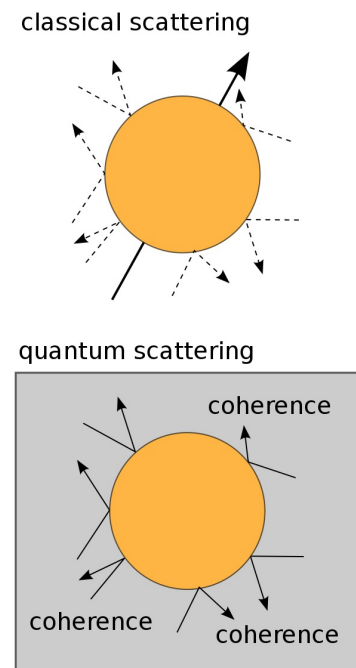
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system to the global combined system-environment pair. Let us consider the example of environmental photons scattering off a particle, which is schematically shown in Fig. 2.1. The classical perturbation to the particle will be determined by the photon momenta, and given the momenta are negligible, environmental effects can be ignored while studying the dynamics of the particle. But in the quantum case, the photons will become entangled with the particle and take away coherence from the system, even if their momenta are virtually zero. This makes superposition of states in some basis determined by the interaction impossible to exist, rendering the system classical. Hence we can not ignore environmental effects while studying the dynamics of quantum systems. In this chapter, we shall see that environmental interactions not only affect the dynamics, but they also decide which observables we see at the system level. The following sections will include a brief study of decoherence in the context of open quantum systems.

2.2 Decoherence and the local damping of interference

In this section, in the context of the double slit experiment, we will show how environmental interaction can lead to the disappearence of interference effects . The environment consists of photons or air molecules that scatter off the electron and hence let us infer the electron's location.
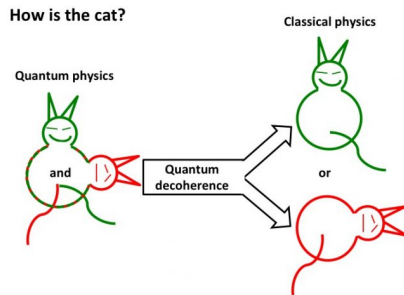

Figure 2.2: Schrödinger's cat turning classical.[Figure taken from: Daniel Moreno Andrés, "Quantum mechanics in biological systems (I): Introduction"]

The number density of these perturbations will vary from one experiment to another and our analysis will let us study its effects at different limits. Let us say that the environment is in the state $|E_0\rangle$ before the interaction takes place and $|\Psi_1\rangle$ and $|\Psi_2\rangle$ represent electron states localized around positions x_1 and x_2, respectively. The interaction dynamics is of the form

$$|\Psi_1\rangle |E_0\rangle \rightarrow |\Psi_1\rangle |E_1\rangle \quad \text{and} \quad |\Psi_2\rangle |E_0\rangle \rightarrow |\Psi_1\rangle |E_2\rangle \tag{2.1}$$

where $|E_1\rangle$ and $|E_2\rangle$ represent post-interaction environmental states. In the double-slit experiment, the pre-

interaction composite state $\left|\Phi^i\right\rangle$ is given by

$$\left|\Phi^i\right\rangle = \frac{1}{\sqrt{2}}\big(\left|\Psi_1\right\rangle + \left|\Psi_2\right\rangle\big)\left|E_0\right\rangle . \tag{2.2}$$

After the interaction takes place, the final composite state $\left|\Phi^f\right\rangle$ becomes of the form

$$\left|\Phi^i\right\rangle \to \left|\Phi^f\right\rangle = \frac{1}{\sqrt{2}}\big(\left|\Psi_1\right\rangle\left|E_1\right\rangle + \left|\Psi_2\right\rangle\left|E_2\right\rangle\big) = \frac{1}{\sqrt{2}}\sum_{i=1}^{2}\left|\Psi_i\right\rangle\left|E_i\right\rangle . \tag{2.3}$$

Now we can find the reduced density matrix of the system and study its properties to understand how the environmental interaction has changed the local dynamics of the electron. Let $\{|e_k\rangle\}$ be an orthonormal basis set of environment. Then, the reduced density matrix of the electron after interaction, $\hat{\rho}^f_{el}$, is given by tracing the full density matrix over the environment states:

$$\hat{\rho}^f_{el} = Tr_{En}\left(\frac{1}{2}\sum_{i,j=1}^{2}\left|\Psi_i\right\rangle\langle\Psi_j|\otimes|E_i\rangle\langle E_j|\right)$$

$$= \frac{1}{2}\sum_{i,j=1}^{2}\left|\Psi_i\right\rangle\langle\Psi_j|\sum_k\langle e_k|E_i\rangle\langle E_j|e_k\rangle$$

$$= \frac{1}{2}\sum_{i,j=1}^{2}\left|\Psi_i\right\rangle\langle\Psi_j|\langle E_j|\left(\sum_k|e_k\rangle\langle e_k|\right)E_i\rangle$$

$$= \frac{1}{2}\sum_{i,j=1}^{2}\left|\Psi_i\right\rangle\langle\Psi_j|\langle E_j|E_i\rangle$$

$$= \frac{1}{2}\big(|\Psi_1\rangle\langle\Psi_1| + |\Psi_2\rangle\langle\Psi_2| + |\Psi_1\rangle\langle\Psi_2|\langle E_2|E_1\rangle + |\Psi_2\rangle\langle\Psi_1|\langle E_1|E_2\rangle\big) . \tag{2.4}$$

The density matrix of the electron before the interaction was given by

$$\hat{\rho}^i_{el} = \frac{1}{2}\big(|\Psi_1\rangle\langle\Psi_1| + |\Psi_2\rangle\langle\Psi_2| + |\Psi_1\rangle\langle\Psi_2| + |\Psi_2\rangle\langle\Psi_1|\big) , \tag{2.5}$$

where the two cross terms at the end denote the interference between the component states $|\Psi_1\rangle$ and $|\Psi_2\rangle$. The effect of the environment on the local dynamics of the system is summarized by the overlap of the environmental states $|E_1\rangle$ and $|E_2\rangle$. This physically corresponds to the distinguishability of the two environmental states which are one-to-one correlated with the component states $|\Psi_1\rangle$ and $|\Psi_2\rangle$. If enough number of particles scatter off the electron, the environmental states correlated with the two different position states of the electron

will be sufficiently distinguishable from one another. For an almost vanishing overlap between these states , i.e., $\langle E_1 | E_2 \rangle \simeq 0$, $\hat{\rho}_{el}^{f}$ becomes

$$\hat{\rho}_{el}^{f} \simeq \frac{1}{2} \big(|\Psi_1\rangle\langle\Psi_1| + |\Psi_2\rangle\langle\Psi_2| \big) . \tag{2.6}$$

The cross terms which represented the interference effects between the component states of the electron have vanished, implying no local observable of the form $\hat{O} = \hat{O}_{el} \otimes \hat{I}_{En}$ can observe interference effects between them. The system has essentially become classical!

Here we have said that the states $|\Psi_1\rangle$ and $|\Psi_2\rangle$ represent states localized around positions x_1 and x_2, but they could have been any two states of the system and, if the interaction between the system and the environment is of the form in Eq. (2.1), the same conclusions will still hold.

2.3 Decoherence timescales

In the previous section, we saw that the vanishing of interference effects between the two states of the system at the system level was a consequence of orthogonality of the environmental states which were one-to-one correlated with them. The orthogonality of the environmental states was motivated from the fact that the system states were sufficiently distinct from one another and that the environment was able to resolve this difference to a good extent. But this decoherence does not happen instantaneously. Let us consider the example of spatial decoherence due to environmental photons scattering off an object. In the long-wavelength limit, i.e., when the separation between x and x' is smaller than the wavelength of the photon, the inner product of the environmental states $\big|E_x(t)\big\rangle$ and $\big|E_{x'}(t)\big\rangle$, which are one-to-one correlated with system states $|\Psi_x\rangle$ and $|\Psi_{x'}\rangle$ denoting localization around x and x', respectively, can be found to be [11]

$$\big\langle E_x(t)\big|E_{x'}(t)\big\rangle = e^{-\Lambda|x-x'|^2 t} = e^{-\frac{t}{\tau_d}} , \tag{2.7}$$

where Λ carries information about the physical properties of the scattering process and τ_d is known as the decoherence timescale. It is the timescale over which the system loses its coherence significantly. The behavior of Eq. (2.7) is quite intuitive. For states that are too close to another, the environment, in the long wavelength limit, can not easily distinguish between them and a lot of photons need to scatter off the object for the environment to be

able to sufficiently resolve the two distinct states, making the decoherence timescale larger. On the other hand, in the short wavelength limit,

$$\left\langle E_x(t) \middle| E_{x'}(t) \right\rangle = e^{-\Gamma t} \, , \tag{2.8}$$

where Γ is the total scattering rate. This behavior can be traced back to the fact that in short wavelength limit, the wavelength of the photon is enough to resolve the separation between x and x' and hence the decoherence timescale is independent of the separation. In summary, decoherence timescales vary from one process to another and largely depend on the nature of interaction between the system and the environment and their properties.

2.4 Einselection and pointer states

Einselection, a shorthand for environment-induced superselection, refers to the dynamical selection of a set of states of the system that are least prone to decoherence. It is in the sense that if the system starts in any one of these states it does not get entangled with the environment and hence does not lose its quantum coherence. Let us say that the interaction between the system and the environment is of the form of Eq. (2.1) and consider two states given by

$$|\Psi_\pm\rangle = \frac{1}{\sqrt{2}} \big(|\Psi_1\rangle \pm |\Psi_2\rangle \big) \, . \tag{2.9}$$

Now if the system starts out in a state $|\Psi\rangle$ which is a superposition of the states $|\Psi_+\rangle$ and $|\Psi_-\rangle$,

$$|\Psi\rangle = \frac{1}{\sqrt{2}} \big(|\Psi_+\rangle + |\Psi_-\rangle \big) \, , \tag{2.10}$$

it does not get entangled with the environment:

$$|\Psi\rangle |E_0\rangle \xrightarrow{Interaction} |\Psi\rangle |E_1\rangle \, . \tag{2.11}$$

This is quite obvious because the state $|\Psi\rangle$ is nothing but the state $|\Psi_1\rangle$. But what is interesting is the fact that the interference effects between components $|\Psi_+\rangle$ and $|\Psi_-\rangle$ are not suppressed by the environmental interaction. We get back the same superposition even after interaction. This, essentially, is the result of the environment's inability to distinguish

between states $|\Psi_+\rangle$ and $|\Psi_-\rangle$. To see this, consider the post-interaction composite state for $|\Psi_\pm\rangle$:

$$|\Psi_\pm\rangle |E_0\rangle \rightarrow \frac{1}{\sqrt{2}} \big(|\Psi_1\rangle |E_1\rangle \pm |\Psi_2\rangle |E_2\rangle \big) . \tag{2.12}$$

Notice that for $\langle\Psi_1|\Psi_2\rangle = 0$, the reduced density matrix associated with the environment for both the states $|\Psi_\pm\rangle$ is

$$\hat{\rho}_E^\pm = \frac{1}{2} \big(|E_1\rangle\langle E_1| + |E_2\rangle\langle E_2| \big) \tag{2.13}$$

Hence no measurement in the $\{|E_1\rangle , |E_2\rangle\}$ basis can reveal any information about which of the states $|\Psi_\pm\rangle$ was prepared initially.

To sum it all up, the states which get minimally entangled with the environment in the course of interaction are known as preferred states or pointer states. These are the states which get minimally affected by decoherence whereas a superposition of such states generally loses its quantum coherence quite rapidly.

If the pointer states are orthogonal to one another and complete, we can say that decoherence leads to the emergence of a preferred basis for the system. For example, in the case of an interaction of the form Eq. (2.1) position eigenstates are the pointer states. As we know that they are complete and orthogonal, position basis is the preferred basis for the system. But there is one small caveat involved. As we know that position eigenstates are not physically realizable, the pointer states are very sharply peaked Gaussians and hence we can say that position basis is an approximate preferred basis for the system.

The emergence of a preferred basis does not always happen. For example, if we consider a spin-half particle interacting with a macroscopic quantum apparatus described by a harmonic oscillator potential which, in turn, is coupled to a heat bath, we can show that at zero temperature of the heat bath, coherent states of the apparatus are the pointer states [3]. But the coherent states are not orthogonal and they form an over-complete basis. Hence, no preferred basis emerges in these cases.

2.5 Finding pointer states

An important part of studying decoherence is to find out the pointer states of the system, given a total Hamiltonian for the combined system-environment pair. One of its prime necessities lie in the domain of quantum information and quantum computation, where we

need states that will be least disturbed by the environmental interaction to perform quantum operations on. We are looking for system states $|s_i\rangle$ of the form

$$|s_i\rangle \left|E_i(0)\right\rangle \to |s_i\rangle \left|E_i(t)\right\rangle \ , \tag{2.14}$$

where $\left|E_i(0)\right\rangle$ and $\left|E_i(t)\right\rangle$ are the environmental states at $t = 0$ and $t = t$, respectively.

In general, the total Hamiltonian is of the form

$$\hat{H}_{total} = \hat{H}_{system} + \hat{H}_{environment} + \hat{H}_{interaction} \ . \tag{2.15}$$

Now we shall try to discuss how to find the pointer states in the quantum measurement limit. Quantum measurement limit is the limit when the energy scales associated with the interaction Hamiltonian is much higher than the energy scales associated with both the system and the environment Hamiltonians. In this limit,

$$\hat{H}_{total} \approx \hat{H}_{interaction} \ . \tag{2.16}$$

Now the interaction Hamiltonian can be written in the form

$$\hat{H}_{int} = \sum_{\alpha} \hat{S}_{\alpha} \otimes \hat{E}_{\alpha} \ , \tag{2.17}$$

where $\{\hat{S}_{\alpha}\}$ and $\{\hat{E}_{\alpha}\}$ are system and environment operators respectively. We claim that Eq. (2.14) will hold for the system states $\{|s_i\rangle\}$ if they are the simultaneous eigenstates of $\{\hat{S}_{\alpha}\}$, i.e.,

$$\hat{S}_{\alpha} |s_i\rangle = \lambda_i^{\alpha} |s_i\rangle \ . \tag{2.18}$$

For such system states, the evolution of the composite state will be given by

$$
\begin{aligned}
e^{-i\hat{H}_{int}t} |s_i\rangle |E_0\rangle &= e^{-i(\sum_{\alpha} \hat{S}_{\alpha} \otimes \hat{E}_{\alpha})t} |s_i\rangle |E_0\rangle \\
&= |s_i\rangle \, e^{-i(\sum_{\alpha} \lambda_i^{\alpha} \hat{E}_{\alpha})t} |E_0\rangle \\
&= |s_i\rangle \left|E_i(t)\right\rangle \ .
\end{aligned}
\tag{2.19}
$$

If the operators $\{\hat{S}_{\alpha}\}$ are Hermitian, they can describe physical observables. Take the example of an interaction Hamiltonian of the form

$$\hat{H} = \hat{x} \otimes \hat{E} \ . \tag{2.20}$$

This could be given a physical meaning that the environment is carrying out a measurement of position of the system. In this case, the position eigenstates will be the pointer states.

One of the main tools for finding the pointer states for a generic total Hamiltonian is known as "the predictability sieve". For finding the predictability sieve for a particular system, we see the evolution of all pure states of the system and employ some measure of mixedness to study which of these states change least by that measure. (An example of such a measure of mixedness of a state would be the von Neumann entropy we introduced in Section 1.5.3.) These states are the ones that retain their quantum nature maximally, i.e., the ones that do not decohere, in the course of their evolution and hence are the approximate pointer states for the system. (Exact pointer states would be the ones that do not change at all due to interaction with the environment. But it is not possible to find such states in many practical situations.) This method is called the predictability sieve because the states that we find are states which are most stable under interactions with environment and hence most predictable.

Chapter 3

Master equations in decoherence

3.1 Introduction

In the previous chapters, we have learned that the information about the local dynamics of the system can be found by studying its reduced density matrix, which is obtained by tracing the total density matrix over the environmental degrees of freedom. Usually, the environment contains a large number of degrees of freedom and it is very difficult to obtain an expression for the density matrix of the total system-environment pair. In the master-equation formalism, certain assumptions are made about the nature of the system-environment interaction and the reduced density matrix at later times is evaluated by

$$\hat{\rho}_S(t) = \hat{O}(t)\hat{\rho}_S(0) \,, \tag{3.1}$$

where $\hat{O}(t)$ is an operator whose form is derived under those assumptions. The best part about this approach is that it enables us to find the approximate evolution of the reduced density matrix of the system even when it is really difficult to find the exact dynamics of the combined state. In this chapter, we shall talk about master equations that are first order differential equations and are local in time, i.e., they are of the form

$$\frac{d}{dt}\hat{\rho}_S(t) = -i[\hat{H}'_S, \hat{\rho}_S(t)] + \hat{D}[\hat{\rho}_S(t)] \,, \tag{3.2}$$

where the first term is the unitary part of the evolution with $\hat{H}'_S$ being the perturbed system Hamiltonian, the free system Hamiltonian perturbed by the environment, and $\hat{D}$ carries information about the non-unitary evolution of the reduced density matrix due to decoherence. In the next section, we will study a very important type of master equation, known as the Born-Markov master equation.

3.2 The Born-Markov master equation

The Born-Markov master equation describes the evolution of the reduced density matrix of the system under two approximations. The approximations are as follows:

1. **Born approximation :** This approximation states that the system is weakly coupled to the environment and the number of degrees of freedom of the environment is large compared to the system. Hence the environmental state remains almost constant during the evolution and the total state can always be written in a product form, i.e.,

$$\hat{\rho}(t) \approx \hat{\rho}_S(t) \otimes \hat{\rho}_E(0) \ . \tag{3.3}$$

2. **Markov approximation :** This approximation states that the correlations that arise within the environment due to its interaction with the system die down much faster than the timescale over which the state of the system undergoes a considerable change. This approximation corresponds to the memory effects of the environment being negligible as the environment quickly "forgets" the information about its interaction with the system.

Now we consider a total Hamiltonian of the form

$$\hat{H} = \hat{H}_0 + \hat{H}_{int} \ , \tag{3.4}$$

where $\hat{H}_0 = \hat{H}_{system} + \hat{H}_{environment}$ and the interaction is treated as a perturbation. Furthermore, it is always possible to write the interaction Hamiltonian $\hat{H}_{int}$ in the diagonalized form

$$\hat{H}_{int} = \sum_{\alpha} \hat{S}_{\alpha} \otimes \hat{E}_{\alpha} \ , \tag{3.5}$$

where $\hat{S}_{\alpha}$ and $\hat{E}_{\alpha}$ are unitary (not necessarily Hermitian) system and environment operators, respectively. Next we introduce the interaction picture, where an operator $\hat{O}(t)$ becomes $\hat{O}^I(t)$ given by

$$\hat{O}^I(t) = e^{i\hat{H}_0 t} \hat{O}(t) e^{-i\hat{H}_0 t} \ . \tag{3.6}$$

The evolution of the density matrix in the interaction picture is given by

$$\frac{d}{dt}\hat{\rho}^I(t) = -i[\hat{H}_{int}, \hat{\rho}^I(t)] \ . \tag{3.7}$$

For such a Hamiltonian, the evolution of the reduced density matrix of the system under the Born-Markov approximation can be found to be [11]

$$\frac{d}{dt}\hat{\rho}_S(t) = -i[\hat{H}_S, \hat{\rho}_S(t)] - \sum_\alpha \left([\hat{S}_\alpha, \hat{B}_\alpha \hat{\rho}_S(t)] + [\hat{\rho}_S(t)\hat{C}_\alpha, \hat{S}_\alpha]\right) , \tag{3.8}$$

where $\hat{B}_\alpha$ and $\hat{C}_\alpha$ are

$$\hat{B}_\alpha = \int_0^\infty d\tau \sum_\beta M_{\alpha\beta}(\tau)\hat{S}_\beta^I(-\tau) \quad \text{and} \quad \hat{C}_\alpha = \int_0^\infty d\tau \sum_\beta M_{\beta\alpha}(-\tau)\hat{S}_\beta^I(-\tau) . \tag{3.9}$$

The quantity $\hat{M}_{\alpha\beta}(\tau)$ is known as the environmental self-correlation function and is given by

$$\hat{M}_{\alpha\beta}(\tau) = \left\langle \hat{E}_\alpha(\tau)\hat{E}_\beta(0) \right\rangle_{\hat{\rho}_E(0)} = Tr_{En}\left(\hat{E}_\alpha(\tau)\hat{E}_\beta(0)\hat{\rho}_E(0)\right) , \tag{3.10}$$

where $\left\langle \hat{O} \right\rangle_{\hat{\rho}_E}$ denotes the expectation value of the operator $\hat{O}$ in the environmental state $\hat{\rho}_E$. The Born-Markov master equation has the important property that it is local in time, i.e., to find the reduced density matrix at a time $t = t + dt$ we only need to know the reduced density matrix at time t. Also, the effect of the environment in the system's dynamics is essentially captured in the coefficients $M_{\alpha\beta}$, where the average is taken over the initial state of the environment.

These are all very desirable features of a master equation but the assumptions we have made to derive this equation are only approximately correct and in some cases the reduced density matrices obtained from Eq. (3.8) violate the positivity condition. The positivity condition is the following. For any density matrix,

$$\hat{\rho} = \sum_i p_i|\Psi_i\rangle\langle\Psi_i| ; \quad p_i \geq 0 , \tag{3.11}$$

$\hat{\rho}$ is always positive in the sense that for any pure state $|\Phi\rangle$,

$$\begin{aligned}
\langle\Phi|\hat{\rho}|\Phi\rangle &= \sum_i p_i \langle\Phi|\Psi_i\rangle \langle\Psi_i|\Phi\rangle \\
&= \sum_i p_i |\langle\Psi_i|\Phi\rangle|^2 \\
&\geq 0 .
\end{aligned} \tag{3.12}$$

The quantity $\langle\Phi|\hat{\rho}|\Phi\rangle$ is interpreted as the occupation probability of the state $|\Phi\rangle$ in $\hat{\rho}$. Hence the negativity of the reduced density matrix of the system is very unphysical. But there exists

a subset of Born-Markov master equations that always respect the positivity of the reduced density matrix of the system. These are the ones that can be written in a form known as the Lindblad form. Note that there are also Born-Markov master equations that cannot be written in the Lindblad form but still respect positivity. We shall discuss the Lindblad form in the next section.

3.3 The Lindblad form

The master equations which can be written in the form [5][4]

$$\frac{d}{dt}\hat{\rho}_S(t) = -i[\hat{H}_s, \hat{\rho}_S(t)] + \frac{1}{2}\sum_{\alpha\beta}\lambda_{\alpha\beta}\big(\,[\hat{S}_\alpha, \hat{\rho}_S(t)\hat{S}_\beta^\dagger] + [\hat{S}_\alpha\hat{\rho}_S(t), \hat{S}_\beta^\dagger]\,\big) \tag{3.13}$$

are known as Lindblad form master equations and they always respect the positivity of the density matrix. The coefficients $\lambda_{\alpha\beta}$ contain all the information about the decoherence process. The matrix defined by the coefficients $\lambda_{\alpha\beta}$ can be diagonalized and the Lindblad form can be transformed into

$$\frac{d}{dt}\hat{\rho}_S(t) = -i[\hat{H}'_s, \hat{\rho}_S(t)] - \frac{1}{2}\sum_{\alpha}c_\alpha\big(\hat{\rho}_S(t)\hat{L}_\alpha^\dagger\hat{L}_\alpha + \hat{L}_\alpha^\dagger\hat{L}_\alpha\hat{\rho}_S(t) - 2\hat{L}_\alpha\hat{\rho}_S(t)\hat{L}_\alpha^\dagger\big)\,, \tag{3.14}$$

where $\hat{H}'_S$ is the perturbed system Hamiltonian, the free system Hamiltonian perturbed by the environment, whereas $\hat{L}_\alpha$s are linear combinations of $\hat{S}_\alpha$ and are known as Lindblad operators or Lindblad generators. As we have stated below Eq. (3.5), the system operators are unitary but not always Hermitian. But when they are, $\hat{L}_\alpha$s are also Hermitian and we can associate observables with them. Then, Eq. (3.14) becomes

$$\frac{d}{dt}\hat{\rho}_S(t) = -i[\hat{H}'_s, \hat{\rho}_S(t)] - \frac{1}{2}\sum_{\alpha}c_\alpha[\hat{L}_\alpha, [\hat{L}_\alpha, \hat{\rho}_S(t)]]\,. \tag{3.15}$$

This final expression has a noticeable consequence in terms of pointer states of the system. If the commutator of $\hat{L}_\alpha$ vanishes with $\hat{\rho}_S(t)$ for all values of α, then the evolution of the density matrix of the system is unitary:

$$\frac{d}{dt}\hat{\rho}_S(t) = -i[\hat{H}'_s, \hat{\rho}_S(t)]\,. \tag{3.16}$$

As $\hat{L}_\alpha$s are nothing but linear combinations of $\hat{S}_\alpha$, in general we would have

$$[\hat{L}_\alpha, \hat{\rho}_S(t)] = 0 \quad \Rightarrow \quad [\hat{S}_\alpha, \hat{\rho}_S(t)] = 0\,. \tag{3.17}$$

We could of course have cases where there are linear combinations of $\hat{S}_\alpha$ that have vanishing commutator with $\hat{\rho}_S(t)$ without $\hat{S}_\alpha$ sharing that property, but such cases would be rare. It is easy to see that the above equation would be satisfied if the system starts out in any of the states $\{|s_i\rangle\}$ which are simultaneous eigen states of all the $\hat{S}_\alpha$,

$$\hat{S}_\alpha |s_i\rangle = \lambda_\alpha^i |s_i\rangle \quad \Rightarrow \quad [\hat{S}_\alpha, \hat{\rho}_S(0)] = \hat{S}_\alpha |s_i\rangle\langle s_i| - |s_i\rangle\langle s_i|\hat{S}_\alpha$$
$$= \lambda_\alpha^i |s_i\rangle\langle s_i| - \lambda_\alpha^i |s_i\rangle\langle s_i|$$
$$= 0 . \tag{3.18}$$

Thus, such states would undergo unitary evolution and would be immune to decoherence in general. Note that this ties in with our earlier statement in Section 2.5 that simultaneous eigenstates of $\{\hat{S}_\alpha\}$ are the pointer states for the system that do not decohere.

Equipped with the understanding of master equations, we shall study a very important type of decoherence model known as the quantum Brownian motion in the next chapter.

Chapter 4

Quantum Brownian motion

4.1 Introduction

In classical physics, Brownian motion is described by the equation

$$m\ddot{x} + \eta\dot{x} + V'(x) = F(t) \, , \tag{4.1}$$

where η is a constant characteristic of damping, $V(x)$ is a potential function and $F(t)$ is a fluctuating force. The force averages out to zero and has a correlation function of the form

$$\langle F(t) \rangle = 0 \quad ; \quad \langle F(t)F(t') \rangle = 2\eta kT\delta(t - t') \, , \tag{4.2}$$

where T is temperature. This form of correlation function is known as white noise (since a Fourier transform of the delta function, to go to the frequency domain, will have equal power at all frequencies). It says that the forces at different times are not correlated with each other. In practical situation, like the case of a particle colliding with ambient molecules, there is a correlation with a certain time scale (since there are interactions between the molecules responsible for the collision) but this timescale is much faster than the other timescales involved in the system and we can effectively take this time scale to be zero. The equations involved in the study of dissipative open quantum systems often take a form similar to the above equation of Brownian motion. In this chapter, we shall study a "particle" q which is coupled to a scalar quantum field ϕ (which is effectively a bunch of harmonic oscillators in Fourier space) and is also bound by a harmonic potential, following the approach taken by Unruh and Zurek in their paper titled *"Reduction of a wave packet in quantum Brownian motion"* [13]. The coordinate q is not a coordinate of the spacetime in which the field lives. It could

be seen as representing some internal degree of freedom of a particle which is permanently located at a fixed point in position space (here taken as the origin).

4.2 The model

The Lagrangian density for this total system is given by [13]

$$\mathscr{L} = \frac{1}{2}\left[\dot{\phi}^2 - \left(\frac{\partial\phi}{\partial x}\right)^2\right] + \frac{\delta(x)}{2}\left(\dot{q}^2 - \Omega_0^2 q^2\right) - \delta(x)\epsilon q\dot{\phi} . \tag{4.3}$$

The first set of terms is the Lagrangian of a free massless scalar field, the second set of terms is the Lagrangian of a harmonic oscillator q (where we have added a $1/2$ factor that we think was missed due to a typo in the paper) and the last term is the interaction term. The constant Ω_0 is the natural frequency of the harmonic oscillator and ϵ is the coupling constant between the system and the field. The δ function signifies that the system represented by q is situated at $x = 0$. We shall see soon that the linear coupling between the field and time-derivative of the coordinate is what gives rise to an equation of the form of a Langevin equation for the coordinate q. Given this Lagrangian density, the conjugate momenta for ϕ and q are

$$\Pi_\phi = \frac{\partial\mathscr{L}}{\partial\dot{\phi}} = \dot{\phi} - \delta(x)\epsilon q , \tag{4.4}$$

$$\Pi_q = \frac{\partial\mathscr{L}}{\partial\dot{q}} = \delta(x)\dot{q} . \tag{4.5}$$

The total energy for the system can be easily found and it is given by

$$E = \int\left[\Pi_\phi\dot{\phi} + \Pi_q\dot{q} - \mathscr{L}\right]dx$$
$$= \frac{1}{2}\left(\dot{q}^2 + \Omega_0^2 q^2\right) + \int\frac{1}{2}\left[\dot{\phi}^2 + \left(\frac{\partial\phi}{\partial x}\right)^2\right]dx , \tag{4.6}$$

which is necessarily a positive-definite quantity. Now we shall turn our attention to finding the evolution equations for ϕ and q. The equation of motion for the field ϕ is

$$\partial_\mu\frac{\partial\mathscr{L}}{\partial\left(\partial_\mu\phi\right)} = \frac{\partial\mathscr{L}}{\partial\phi} \quad\text{for}\quad \mu = x, t \Rightarrow \partial_t\left(\dot{\phi} - \epsilon\delta(x)q\right) + \partial_x\left(-\partial_x\phi\right) = 0$$
$$\Rightarrow \ddot{\phi} - \partial_x^2\phi = \epsilon\delta(x)\dot{q} . \tag{4.7}$$

On the other hand, the equation of motion for q is given by

$$\partial_t\left(\frac{\partial\mathscr{L}}{\partial\dot{q}}\right) = \frac{\partial\mathscr{L}}{\partial q} \Rightarrow \ddot{q} + \Omega_0^2 q = -\epsilon\dot{\phi}\Big|_{x=0} . \tag{4.8}$$

The delta function is responsible for the value of the field at only $x = 0$ to be present on the right hand side.

Eq. (4.7) has the solution

$$\phi = \phi_1 \equiv \phi_0 + \frac{\epsilon}{2} \left[q(t-x)\theta(x) + q(t+x)\theta(-x) \right] , \tag{4.9}$$

where $\theta(x)$ is the Heaviside function and ϕ_0 is the complementary function for Eq. (4.7), i.e.,

$$\ddot{\phi}_0 - \partial_x^2 \phi_0 = 0 . \tag{4.10}$$

We shall assume that ϕ_0 is chosen as infinitely differentiable. Note that this solution can be equivalently written as

$$\phi_1 = \phi_0 + \frac{\epsilon}{2} q(t - |x|) \equiv \phi_0 + \frac{\epsilon}{2} q(v) . \tag{4.11}$$

Since $|x|$ is continuous function, this is also continuous. Taking the time derivative,

$$\frac{\partial \phi_1}{\partial t} = \dot{\phi}_0 + \frac{\epsilon}{2} \frac{\partial q(v)}{\partial v} = \dot{\phi}_0 + \frac{\epsilon}{2} \dot{q}(t - |x|) , \tag{4.12}$$

which, assuming the function q has continuous first derivatives, is continuous. Here, the $\dot{q}(t - |x|)$ in the last line has to be interpreted as the object obtained by taking the first derivative of the function $q(t)$ and then replacing t by $t - |x|$ in the resulting expression. Similarly, all higher time derivatives are continuous if the corresponding derivatives of q are continuous. Next we take the first spatial derivative:

$$\frac{\partial \phi_1}{\partial x} = \frac{\partial \phi_0}{\partial x} - \frac{\epsilon}{2} \frac{\partial q(v)}{\partial v} \frac{\partial |x|}{\partial x} = \frac{\partial \phi_0}{\partial x} - \frac{\epsilon}{2} \frac{\partial q(v)}{\partial v} \left[\theta(x) - \theta(-x) \right] , \tag{4.13}$$

which is discontinuous only at $x = 0$, again assuming that the first derivative of the function q is continuous. Taking one more spatial derivative,

$$\begin{aligned}
\frac{\partial^2 \phi_1}{\partial x^2} &= \frac{\partial^2 \phi_0}{\partial x^2} - \frac{\epsilon}{2} \frac{\partial^2 q(v)}{\partial v^2} \left[\theta(x) - \theta(-x) \right]^2 - \frac{\epsilon}{2} \frac{\partial q(v)}{\partial v} \left[\delta(x) + \delta(-x) \right] \\
&= \frac{\partial^2 \phi_0}{\partial x^2} - \frac{\epsilon}{2} \frac{\partial^2 q(v)}{\partial v^2} - \epsilon \frac{\partial q(v)}{\partial v} \delta(x) \\
&= \frac{\partial^2 \phi_0}{\partial x^2} - \frac{\epsilon}{2} \frac{\partial^2 q(v)}{\partial v^2} - \epsilon \dot{q} \delta(x) \quad \text{where} \quad \dot{q} = \frac{\partial q(t)}{\partial t} ,
\end{aligned} \tag{4.14}$$

Here the delta function gives the size of the discontinuity in the first derivative along x.

Now we shall show that Eq. (4.7) can be solved by Eq. (4.9).

Proof: From Eq. (4.9), we can see that

$$\phi_1 = \phi_0 + \frac{\epsilon}{2} q(t - x) \quad \text{for} \quad x > 0 \,, \tag{4.15a}$$

$$\phi_1 = \phi_0 + \frac{\epsilon}{2} q(t + x) \quad \text{for} \quad x < 0 \,. \tag{4.15b}$$

Now,

$$\ddot{q}\,(t \pm x) - \partial_x^2 q(t \pm x) = 0 \,. \tag{4.16}$$

So, for $x \neq 0$,

$$\ddot{\phi}_1 - \partial_x^2 \phi_1 = \ddot{\phi}_0 - \partial_x^2 \phi_0 + \frac{\epsilon}{2}\left[\ddot{q}\,(t \pm x) - \partial_x^2 q(t \pm x)\right] = 0 \,, \tag{4.17}$$

which means that Eq. (4.9) satisfies Eq. (4.7) for $x \neq 0$. The effect of the delta function on the right hand side of Eq. (4.7) is that it fixes the amount of discontinuity in $\partial_x \phi$ at the origin. Integrating Eq. (4.7) with respect to x infinitesimally about the origin, we find

$$\lim_{a \to 0^+}\left[\int_{-a}^{a} \ddot{\phi}\, dx - \left.\frac{\partial \phi}{\partial x}\right|_{-a}^{a}\right] = \epsilon \dot{q} \,. \tag{4.18}$$

The first term on the LHS of the above equation vanishes for any well-behaved function and we are left with

$$\lim_{a \to 0^+}\left[\left.\frac{\partial \phi}{\partial x}\right|_{a} - \left.\frac{\partial \phi}{\partial x}\right|_{-a}\right] = -\epsilon \dot{q} \,. \tag{4.19}$$

Let us evaluate this quantity for Eq. (4.9).

$$\lim_{a \to 0^+}\left.\frac{\partial \phi_1}{\partial x}\right|_{a} = \lim_{a \to 0^+}\left[\left.\frac{\partial \phi_0}{\partial x}\right|_{a} - \frac{\epsilon}{2}\dot{q}(t - x)\bigg|_{a}\right] = \lim_{a \to 0^+}\left.\frac{\partial \phi_0}{\partial x}\right|_{a} - \frac{\epsilon}{2}\dot{q}(t) \,, \tag{4.20}$$

$$\lim_{a \to 0^+}\left.\frac{\partial \phi_1}{\partial x}\right|_{-a} = \lim_{a \to 0^+}\left[\left.\frac{\partial \phi_0}{\partial x}\right|_{-a} + \frac{\epsilon}{2}\dot{q}(t + x)\bigg|_{-a}\right] = \lim_{a \to 0^+}\left.\frac{\partial \phi_0}{\partial x}\right|_{-a} + \frac{\epsilon}{2}\dot{q}(t) \,. \tag{4.21}$$

Remembering that ϕ_0 and all its derivatives are continuous, we find

$$\lim_{a \to 0^+}\left[\left.\frac{\partial \phi_1}{\partial x}\right|_{a} - \left.\frac{\partial \phi_1}{\partial x}\right|_{-a}\right] = -\epsilon \dot{q} \,, \tag{4.22}$$

which is what the delta function contribution in Eq. (4.14) is. Hence we can finally conclude that Eq. (4.9) is a solution of Eq. (4.7).

We can now substitute this solution in Eq. (4.8). Using Eq. (4.12), we find

$$\ddot{q} + \frac{\epsilon^2}{2}\dot{q} + \Omega_0^2 q = -\epsilon\dot{\phi}_0 \,, \tag{4.23}$$

to be evaluated at $x = 0$. This equation is of the form of the classic Langevin equation for the coordinate q with the free field ϕ_0 playing the role of the forcing term. Let us solve this equation to find the general form of q at any time t.

The complementary function q_c for the differential equation given by Eq. (4.23) is easy to find. Taking a trial solution of the form $q = e^{\alpha t}$ for the equation

$$\ddot{q}_c + \frac{\epsilon^2}{2}\dot{q}_c + \Omega_0^2 q_c = 0 \tag{4.24}$$

yields

$$\alpha^2 + \frac{\epsilon^2}{2}\alpha + \Omega_0^2 = 0 \,, \tag{4.25}$$

which together with the fact that q_0 and p_0 are the initial position and momenta of the particle gives us

$$q_c = \left[q_0 \cos \Omega t + (p_0 + \gamma q_0) \sin \Omega T / \Omega\right] e^{-\gamma t} \,, \tag{4.26}$$

where we have defined

$$\gamma = \frac{\epsilon^2}{4} \quad ; \quad \Omega = \sqrt{\Omega_0^2 - \gamma^2} \,. \tag{4.27}$$

Now to get the particular integral of Eq. (4.23) we shall first find the Green's function $G(t, t')$ satisfying

$$\ddot{G}(t, t') + 2\gamma\dot{G}(t, t') + \Omega_0^2 G(t, t') = \delta(t - t') = \frac{1}{2\pi} \int_{-\infty}^{\infty} d\omega e^{i\omega(t-t')} \,. \tag{4.28}$$

Using the D operator method, where $D \equiv \frac{d}{dt}$ yields

$$
\begin{aligned}
G(t, t') &= \frac{1}{2\pi} \int_{-\infty}^{\infty} d\omega \, \frac{e^{i\omega(t-t')}}{D^2 + 2\gamma D + \Omega_0^2} \\
&= \frac{1}{2\pi} \int_{-\infty}^{\infty} d\omega \, \frac{e^{i\omega(t-t')}}{-\omega^2 + 2i\omega\gamma + \Omega_0^2} \\
&= \frac{1}{2\pi} \int_{-\infty}^{\infty} d\omega \, \frac{e^{i\omega(t-t')}}{\left[\omega - (i\gamma - \Omega)\right]\left[(\Omega + i\gamma) - \omega\right]} \,.
\end{aligned}
\tag{4.29}
$$

This integral can be evaluated using contour integral methods. The integral has two simple poles in the upper half plane and for $t > t'$, i.e., $(t - t') > 0$, using the residue theorem, it can be written as [8]

$$G(t, t') = \frac{1}{2\pi} \times 2\pi i \times \sum \text{Residues of the integral in the upper half plane}$$

$$= i \left[\frac{e^{i(i\gamma-\Omega)(t-t')}}{2\Omega} - \frac{e^{i(i\gamma+\Omega)(t-t')}}{2\Omega} \right]$$

$$= \frac{e^{-\gamma(t-t')}}{\Omega} \left[\frac{e^{i\Omega(t-t')} - e^{-i\Omega(t-t')}}{2i} \right]$$

$$= \frac{1}{\Omega} \sin \left[\Omega(t-t') \right] e^{-\gamma(t-t')} . \tag{4.30}$$

And, as for $t < t'$, i.e., $(t - t') < 0$,

$$G(t, t') = \frac{1}{2\pi} \times 2\pi i \times \sum \text{Residues of the integral in the lower half plane} = 0 . \tag{4.31}$$

Now the particular integral q_p for Eq. (4.23) can be written as

$$q_p = \int_0^\infty G(t, t') \left[-\epsilon \dot{\phi}_0(t') \right] dt' = -\frac{\epsilon}{\Omega} \int_0^t dt' \, \sin \left[\Omega(t - t') \right] e^{-\gamma(t-t')} \dot{\phi}_0(t') . \tag{4.32}$$

Hence, the entire solution for Eq. (4.23) is

$$q = q_c + q_p = \left[q_0 \cos \Omega t + (p_0 + \gamma q_0) \sin \Omega t / \Omega \right] e^{-\gamma t} - \frac{\epsilon}{\Omega} \int_0^t dt' \, \sin \left[\Omega(t - t') \right] e^{-\gamma(t-t')} \dot{\phi}_0(t') . \tag{4.33}$$

The momentum p, from Eq. (4.5), is

$$p = \dot{q} = \left[p_0 \cos \Omega t - \left[\frac{\gamma}{\Omega} (p_0 + \gamma q_0) + \Omega q_0 \right] \sin \Omega t \right] e^{-\gamma t}$$

$$- \frac{\epsilon}{\Omega} \frac{d}{dt} \int_0^t dt' \, \sin \left[\Omega(t - t') \right] e^{-\gamma(t-t')} \dot{\phi}_0(t') . \tag{4.34}$$

The above set of equations can describe classical as well as quantum systems and hence we can treat q, p, ϕ as operators as well. When position and momentum are used as operators, we shall use the notation P, Q.

The state of the total system is described by the density matrix ρ_{OF}, whereas the state of the oscillator alone is described by the reduced density matrix ρ:

$$\rho \equiv \rho_O = \text{Tr}_F(\rho_{OF}) . \tag{4.35}$$

We introduce a "(k, Δ)" representation for the density matrix as

$$\rho(k, \Delta) = \int dq' \, e^{ikq'} \rho(q' - \Delta/2, q' + \Delta/2) . \tag{4.36}$$

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Next we represent the position components of the density matrix using shift operators $e^{ip\Delta}$. Notice that

$$
\begin{aligned}
\text{Tr}\left[\delta(Q-q)e^{ip\Delta/2}\rho e^{ip\Delta/2}\right] &= \int d\tilde{Q}\langle\tilde{Q}|\delta(Q-q)e^{ip\Delta/2}\rho e^{ip\Delta/2}|\tilde{Q}\rangle \\
&= \int d\tilde{Q}\delta(\tilde{Q}-q)\langle\tilde{Q}|e^{ip\Delta/2}\rho e^{ip\Delta/2}|\tilde{Q}\rangle \\
&= \int d\tilde{Q}\delta(\tilde{Q}-q)\langle\tilde{Q}-\Delta/2|\rho|\tilde{Q}+\Delta/2\rangle \quad \text{as} \quad e^{ip\Delta}\left|\tilde{Q}\right\rangle = \left|\tilde{Q}+\Delta\right\rangle \\
&= \langle q-\Delta/2|\rho|q+\Delta/2\rangle \\
&= \rho(q-\Delta/2, q+\Delta/2) .
\end{aligned}
$$
(4.37)

where we have denoted the eigenvalue of Q associated with the eigenstate $\left|\tilde{Q}\right\rangle$ as $\tilde{Q}$ to avoid confusion between the operator Q and its eigenvalue, i.e.,

$$
Q\left|\tilde{Q}\right\rangle = \tilde{Q}\left|\tilde{Q}\right\rangle
$$
(4.38)

We can now derive an expression for $\rho(k,\Delta)$ in terms of the density matrix, position and momentum operators:

$$
\begin{aligned}
\rho(k,\Delta) &= \int dq' \, e^{ikq'}\rho(q'-\Delta/2, q'+\Delta/2) \\
&= \int dq' \, e^{ikq'}Tr\left[\delta(Q-q')e^{ip\Delta/2}\rho e^{ip\Delta/2}\right] \\
&= \int dq' \, d\tilde{Q}e^{ikq'}\delta(\tilde{Q}-q')\langle\tilde{Q}|e^{ip\Delta/2}\rho e^{ip\Delta/2}|\tilde{Q}\rangle \\
&= \int d\tilde{Q} \, e^{ik\tilde{Q}}\langle\tilde{Q}|e^{ip\Delta/2}\rho e^{ip\Delta/2}|\tilde{Q}\rangle \\
&= \int d\tilde{Q} \, \langle\tilde{Q}|e^{ikQ}e^{ip\Delta/2}\rho e^{ip\Delta/2}|\tilde{Q}\rangle \\
&= \int d\tilde{Q} \, \langle\tilde{Q}|e^{i\left(kQ+\Delta P/2\right)}e^{-\frac{ik\Delta}{4}}\rho e^{ip\Delta/2}|\tilde{Q}\rangle \quad \text{[using B.C.H formula [10] , } [Q,P]=i\text{]} \\
&= \int d\tilde{Q} \, e^{-\frac{ik\Delta}{4}}\langle\tilde{Q}|e^{ip\Delta/2}e^{i\left(kQ+\Delta P/2\right)}\rho|\tilde{Q}\rangle \quad \text{[using cyclicity of trace]} \\
&= \int d\tilde{Q} \, e^{-\frac{ik\Delta}{4}}e^{\frac{ik\Delta}{4}}\langle\tilde{Q}|e^{i(kQ+\Delta P)}\rho|\tilde{Q}\rangle \\
&= \text{Tr}\left[e^{i(kQ+\Delta P)}\rho\right]
\end{aligned}
$$
(4.39)

While working in the Heisenberg representation, the density matrix remains constant while the operators change with time. We have the functional form of $Q(t)$ and $P(t)$ in Eq. (4.33)

and Eq. (4.34), respectively. Plugging those in Eq. (4.39) and assuming that the system and the field were uncorrelated at $t = 0$ yields

$$
\rho(k, \Delta) = \text{Tr}\left[\rho^0 e^{i\left[\Delta\left(P_0 \cos \Omega t - \frac{\gamma}{\Omega} P_0 \sin \Omega t - \frac{\gamma^2 + \Omega^2}{\Omega} Q_0 \sin \Omega t\right)e^{-\gamma t} + k\left(Q_0 \cos \Omega t + \frac{P_0 + \gamma Q_0}{\Omega} \sin \Omega t\right)e^{-\gamma t}\right]}\right.
$$
$$
\left. \times \text{Tr}_F\left[\rho_F^0 \exp\left\{-i\left[\Delta \frac{d}{dt} + k\right]\frac{\epsilon}{\Omega}\int_0^t \sin\left(\Omega(t - t')\right)e^{-\gamma(t - t')}dt'\right\}\right]\right]. \tag{4.40}
$$

where we have taken

$$
\rho^0 \equiv \rho_O^0 \quad \text{and} \quad \rho_{OF}^0 = \rho^0 \rho_F^0 . \tag{4.41}
$$

The right hand side of Eq. (4.40) has been obtained in the Heisenberg picture where the operators had been taken to time dependent. But we can connect with the Schrödinger picture where k, Δ will be time dependent using the relation

$$
\rho(k, \Delta) = \rho^0(k(t), \Delta(t))E(k, \Delta; t) , \tag{4.42}
$$

where $E(k, \Delta; t)$ denotes the effect of environment on $\rho(k, \Delta)$. Now,

$$
\rho^0(k(t), \Delta(t)) = \text{Tr}\left[\exp\{i(k(t)Q_0 + \Delta(t)P_0)\}\rho_0\right] . \tag{4.43}
$$

Hence Eq. (4.42) can be written as

$$
\rho(k, \Delta) = \rho^0(k(t), \Delta(t))E(k, \Delta; t)
$$
$$
= \text{Tr}\left[\exp\{i(k(t)Q_0 + \Delta(t)P_0)\}\rho_0\right] E(k, \Delta; t) . \tag{4.44}
$$

Comparing this with Eq. (4.40) and rearranging terms results in

$$
\Delta(t) = \left[\Delta\left[\cos \Omega t - \frac{\gamma}{\Omega}\sin \Omega t\right] + \frac{k}{\Omega}\sin \Omega t\right]e^{-\gamma t}, \tag{4.45a}
$$

$$
k(t) = \left[k\left[\cos \Omega t + \frac{\gamma}{\Omega}\sin \Omega t\right] - \frac{\Delta(\gamma^2 + \Omega^2)}{\Omega}\sin \Omega t\right]e^{-\gamma t}, \tag{4.45b}
$$

$$
E(k, \Delta; t) = \text{Tr}_F\left[\rho_F^0 \exp\left\{-i\left[\Delta \frac{d}{dt} + k\right]\frac{\epsilon}{\Omega}\int_0^t \sin\left(\Omega(t - t')\right)e^{-\gamma(t - t')}dt'\right\}\right] . \tag{4.45c}
$$

The kernel for the evolution of the density matrix is simply

$$
G(k', \Delta', k, \Delta; t) = \delta(k' - k(t))\delta(\Delta' - \Delta(t))E(k', \Delta'; t) , \tag{4.46}
$$

as

$$\int dk' \, d\Delta' \, G(k', \Delta', k, \Delta; t)\rho^0(k', \Delta') = \rho^0(k(t), \Delta(t))E(k, \Delta; t) = \rho(k, \Delta) \ . \tag{4.47}$$

Eq. (4.44) along with Eq. (4.45c) give the complete solution for the reduced density matrix of the system.

4.3 The master equation

In the previous section, we obtained the full solution for the reduced density matrix of the system. Here we shall obtain the master equation that governs the evolution of the reduced density matrix. We shall do so because the master equation shows different effects of the environment on the system (such as dissipation, decoherence, etc.) and often it is easier to numerically integrate the master equation than to evaluate the solution numerically.

The master equation is of the form

$$\dot{\rho} = L\rho \ . \tag{4.48}$$

In order to find the operator L which generates time evolution, we need to find the time derivative of $\rho(k, \Delta)$. For this purpose, we shall use the formula that for any operator $A(t)$

$$\frac{de^{A(t)}}{dt} = \int_0^1 e^{\lambda A(t)} \dot{A} e^{(1-\lambda)A(t)} d\lambda \ . \tag{4.49}$$

The expression for reduced density matrix is

$$\mathrm{Tr}\left[\rho^0 e^{i(kQ+\Delta P)}\right] \ . \tag{4.50}$$

Differentiating this equation with respect to time gives

$$\dot{\rho} = \mathrm{Tr}\left[\rho^0 \int_0^1 e^{i\lambda(kQ+\Delta P)}[i(k\dot{Q} + \Delta \dot{p})]e^{i(1-\lambda)(kQ+\Delta P)}d\lambda\right] \ . \tag{4.51}$$

Now we use $\dot{Q} = P$ and evaluate $\dot{P} = \ddot{Q}$ using Eq. (4.8). Plugging these in the above equation leads to

$$\dot{\rho} = \mathrm{Tr}\left[\rho^0 \int_0^1 e^{i\lambda(kQ+\Delta P)}[i(kP + \Delta(-\Omega_0^2 Q - \epsilon^2 P/2 - \epsilon\dot{\phi}_0))]e^{i(1-\lambda)(kQ+\Delta P)}d\lambda\right] \ . \tag{4.52}$$

To simplify this equation, we shall use the derivatives of $\rho(k, \Delta)$ w.r.t (k, Δ). They are found to be

$$\frac{\partial \rho(k, \Delta)}{\partial \Delta} = \text{Tr} \left[\rho^0 \int_0^1 e^{i\lambda(kQ+\Delta P)} [iP] e^{i(1-\lambda)(kQ+\Delta P)} d\lambda \right] , \tag{4.53}$$

$$\frac{\partial \rho(k, \Delta)}{\partial k} = \text{Tr} \left[\rho^0 \int_0^1 e^{i\lambda(kQ+\Delta P)} [iQ] e^{i(1-\lambda)(kQ+\Delta P)} d\lambda \right] . \tag{4.54}$$

Using the above two equations, Eq. (4.52) simplifies to

$$\dot\rho = \left[k\frac{\partial}{\partial \Delta} - \Delta\Omega_0^2 \frac{\partial}{\partial k} - \frac{\Delta\epsilon^2}{2} \frac{\partial}{\partial \Delta} \right] \rho(k, \Delta) - i\Delta\epsilon \text{Tr} \left[\rho^0 \int_0^1 e^{i\lambda(kQ+\Delta P)} \dot\phi_0 e^{i(1-\lambda)(kQ+\Delta P)} d\lambda \right] . \tag{4.55}$$

Let us denote the second part of this equation by $D(t)$, i.e.,

$$D(t) = -i\Delta\epsilon \, \text{Tr} \left[\rho^0 \int_0^1 e^{i\lambda(kQ+\Delta P)} \dot\phi_0 e^{i(1-\lambda)(kQ+\Delta P)} d\lambda \right] . \tag{4.56}$$

We need to find a simplified form of $D(t)$ and to do so we first calculate

$kQ + \Delta P$

$$= k\left(Q_0 \cos\Omega t + \frac{P_0 + \gamma Q_0}{\Omega} \sin\Omega t \right) e^{-\gamma t} + \Delta \left(P_0 \cos\Omega t - \left[\frac{\gamma}{\Omega}(P_0 + \gamma Q_0) + \Omega Q_0 \right] \sin\Omega t \right) e^{-\gamma t}$$

$$- \left(\Delta\frac{d}{dt} + k \right) \left[\frac{\epsilon}{\Omega} \int_0^t dt' \, \sin(\Omega(t - t')) e^{-\gamma(t-t')} \dot\phi_0(t') \right] . \tag{4.57}$$

For the sake of notational clarity, we define $\Psi(t)$, which is a function of the field ϕ as well as time, as

$$\Psi(t) = \left[\frac{\epsilon}{\Omega} \int_0^t dt' \, \sin(\Omega(t - t')) e^{-\gamma(t-t')} \dot\phi_0(t') \right] . \tag{4.58}$$

We also denote the ϕ independent part as $S(k, \Delta, P_0, Q_0)$, i.e.,

$$S(k, \Delta, P_0, Q_0) = k\left(Q_0 \cos\Omega t + \frac{P_0 + \gamma Q_0}{\Omega} \sin\Omega t \right) e^{-\gamma t}$$

$$+ \Delta \left(P_0 \cos\Omega t - \left[\frac{\gamma}{\Omega}(P_0 + \gamma Q_0) + \Omega Q_0 \right] \sin\Omega t \right) e^{-\gamma t} . \tag{4.59}$$

With this notation, $D(t)$ becomes

$$D(t) = -i\Delta\epsilon \operatorname{Tr}\left[\rho^0 \int_0^1 e^{i\lambda(S(k,\Delta,P_0,Q_0)-(\Delta d/dt+k)\Psi(t))}\dot{\phi}_0 e^{i(1-\lambda)(S(k,\Delta,P_0,Q_0)-(\Delta d/dt+k)\Psi(t))}d\lambda\right].$$
(4.60)

Noticing that $S(k,\Delta,P_0,Q_0)$ commutes with $\dot{\phi}_0$, we get

$$D(t) = -i\Delta\epsilon \operatorname{Tr}\left[\rho^0 e^{i(S(k,\Delta,P_0,Q_0))}\right]$$

$$\times \operatorname{Tr}\left[\rho_F^0 \int_0^1 d\lambda \left[\exp\left\{-i\lambda(k+\Delta\frac{d}{dt})\Psi(t)\right\}\dot{\phi}_0 \exp\left\{-i(1-\lambda)(k+\Delta\frac{d}{dt})\Psi(t)\right\}\right]\right].$$
(4.61)

Now the expression for $\rho(k,\Delta)$ from Eq. (4.40) can be written as

$$\rho(k,\Delta) = \operatorname{Tr}\left[\rho^0 e^{i(S(k,\Delta,P_0,Q_0))}\right] \operatorname{Tr}\left[\rho_F^0 \exp\left\{-i(k+\Delta\frac{d}{dt})\Psi(t)\right\}\right].$$
(4.62)

We shall now show that $D(t)$ can be written as

$$D(t) = -i\Delta\epsilon\rho(k,\Delta) \left[-i\frac{\partial}{\partial\alpha}\ln \operatorname{Tr}\left[\rho_F^0 \exp\left\{-i\left[(k+\Delta\frac{d}{dt})\Psi(t)-\alpha\dot{\phi}_0\right]\right\}\right]\right]\Bigg|_{\alpha=0}.$$
(4.63)

Consider the quantity,

$$\frac{\partial}{\partial\alpha}\ln\operatorname{Tr}\left[\rho_F^0 \exp\left\{-i\left[(k+\Delta\frac{d}{dt})\Psi(t)-\alpha\dot{\phi}_0\right]\right\}\right]\Bigg|_{\alpha=0} \equiv \frac{\partial}{\partial\alpha}\ln\mathscr{M}\Bigg|_{\alpha=0}$$

$$= \operatorname{Tr}\left[\rho_F^0 \int_0^1 d\lambda \exp\left\{-i\lambda\left[(k+\Delta\frac{d}{dt})\Psi(t)-\alpha\dot{\phi}_0\right]\right\}\left[i\dot{\phi}_0\right]\right.$$

$$\left. \times \exp\left\{-i(1-\lambda)\left[(k+\Delta\frac{d}{dt})\Psi(t)-\alpha\dot{\phi}_0\right]\right\}\right] \times \mathscr{M}^{-1}\Bigg|_{\alpha=0}$$

$$= \operatorname{Tr}\left[\rho_F^0 \int_0^1 d\lambda \exp\left\{-i\lambda\left[(k+\Delta\frac{d}{dt})\Psi(t)\right]\right\}\left[i\dot{\phi}_0\right]\right.$$

$$\left. \times \exp\left\{-i(1-\lambda)\left[(k+\Delta\frac{d}{dt})\Psi(t)\right]\right\}\right] \times \mathscr{M}^{-1}.$$
(4.64)

Using this, the right hand side of Eq. (4.63) becomes

$$-i\Delta\epsilon\rho(k,\Delta) \left[-i\frac{\partial}{\partial\alpha}\ln \operatorname{Tr}\left[\rho_F^0 \exp\left\{-i\left[(k+\Delta\frac{d}{dt})\Psi(t)-\alpha\dot{\phi}_0\right]\right\}\right]\right]\Bigg|_{\alpha=0}$$

$$= -i\Delta\epsilon \mathrm{Tr}\left[\rho^0 e^{i(S(k,\Delta,P_0,Q_0))}\right] \times \mathscr{M} \times (-i)$$

$$\times \mathrm{Tr}\left[\rho_F^0 \int_0^1 d\lambda \exp\left\{-i\lambda\left[(k+\Delta\frac{d}{dt})\Psi(t)\right]\right\}\left[i\dot{\phi}_0\right]\exp\left\{-i(1-\lambda)\left[(k+\Delta\frac{d}{dt})\Psi(t)\right]\right\}\right]\mathscr{M}^{-1}$$

$$= -i\Delta\epsilon\ \mathrm{Tr}\left[\rho^0 e^{i(S(k,\Delta,P_0,Q_0))}\right]$$

$$\times \mathrm{Tr}\left[\rho_F^0 \int_0^1 d\lambda\left[\exp\left\{-i\lambda(k+\Delta\frac{d}{dt})\Psi(t)\right\}\dot{\phi}_0\exp\left\{-i(1-\lambda)(k+\Delta\frac{d}{dt})\Psi(t)\right\}\right]\right]$$

$$= D(t)\ . \quad \text{[Q.E.D]} \tag{4.65}$$

Now, for any arbitrary linear operator O and a Gaussian density matrix ρ,

$$\mathrm{Tr}\left[\rho_F^0 \exp\{iO\phi_0\}\right] = \exp\left\{-\frac{1}{2}Tr\left[\rho_F^0(O\phi_0^2)\right]\right\}. \tag{4.66}$$

Inspecting Eq. (4.63), we find that it is of the form

$$D(t) = -i\Delta\epsilon\rho(k,\Delta)\left[-i\frac{\partial}{\partial\alpha}\ln\mathrm{Tr}\left[\rho_F^0 \exp\{iO\phi_0\}\right]\right]\Bigg|_{\alpha=0}, \tag{4.67}$$

where,

$$O\phi_0 = -(k+\Delta\frac{d}{dt})\Psi(t) + \alpha\dot{\phi}_0\ . \tag{4.68}$$

Now we are in a position to obtain a simpler expression for $D(t)$. Notice that

$$D(t) = -i\Delta\epsilon\rho(k,\Delta)\left[-i\frac{\partial}{\partial\alpha}\ln\mathrm{Tr}\left[\rho_F^0 \exp\{iO\phi_0\}\right]\right]\Bigg|_{\alpha=0}$$

$$= -i\Delta\epsilon\rho(k,\Delta)\left[-i\frac{\partial}{\partial\alpha}\ln\ \exp\left\{-\frac{1}{2}Tr\left[\rho_F^0(O\phi_0^2)\right]\right\}\right]\Bigg|_{\alpha=0}$$

$$= \frac{\Delta\epsilon\rho}{2}\frac{\partial}{\partial\alpha}\mathrm{Tr}\left[\rho_F^0(O\phi_0^2)\right]\Bigg|_{\alpha=0}$$

$$= \frac{\Delta\epsilon\rho}{2}\mathrm{Tr}\left[\rho_F^0\frac{\partial}{\partial\alpha}(O\phi_0^2)\right]\Bigg|_{\alpha=0}$$

$$= \frac{\Delta\epsilon\rho}{2}\mathrm{Tr}\left[\rho_F^0\frac{\partial}{\partial\alpha}\left[-2\left(\alpha\dot{\phi}_0(t)\right)\left(k+\Delta\frac{d}{dt}\right)\Psi(t)+\alpha^2\dot{\phi}_0^2(t)\right]\right]\Bigg|_{\alpha=0}$$

$$= \frac{\Delta\epsilon\rho}{2}\mathrm{Tr}\left[\rho_F^0\left[-2\dot{\phi}_0(t)\left(k+\Delta\frac{d}{dt}\right)\Psi(t)\right]\right]$$

$$= -\Delta\epsilon\rho\ \mathrm{Tr}\left[\rho_F^0\ \dot{\phi}_0(t)\left(k+\Delta\frac{d}{dt}\right)\frac{\epsilon}{\Omega}\int_0^t dt'\ \sin\left(\Omega(t-t')\right)e^{-\gamma(t-t')}\dot{\phi}_0(t')\right] \quad ;\tau\equiv t-t'$$

$$= -\Delta\epsilon\rho \operatorname{Tr}\left[\rho_F^0 \dot{\phi}_0(t)\left[k\Psi(t) + \frac{\Delta\epsilon}{\Omega}\int_0^t dt'\left[\Omega\cos\Omega\tau e^{-\gamma\tau} - \gamma\sin\Omega t e^{-\gamma\tau}\right]\dot{\phi}_0(t')\right]\right]$$

$$= -\Delta\epsilon^2\rho \operatorname{Tr}\left[\rho_F^0\left[(k-\gamma\Delta)\int_0^t dt'\, \frac{\sin\Omega\tau}{\Omega}e^{-\gamma\tau}\dot{\phi}_0(t)\dot{\phi}_0(t')\right.\right.$$

$$\left.\left. + \Delta\int_0^t dt'\,\cos\Omega\tau e^{-\gamma\tau}\dot{\phi}_0(t)\dot{\phi}_0(t')\right]\right] . \tag{4.69}$$

Due to the requirement of symmetrization,

$$\operatorname{Tr}\left[\rho_F^0\dot{\phi}_0(t)\dot{\phi}_0(t')\right] = \frac{1}{2}\langle\dot{\phi}_0(t)\dot{\phi}_0(t') + \dot{\phi}_0(t')\dot{\phi}_0(t)\rangle_{\rho_F} . \tag{4.70}$$

Using this in Eq. (4.69) yields

$$D(t) = -\frac{\Delta\epsilon^2}{2}\rho(k,\Delta)\left[(k-\gamma\Delta)\int_0^t dt'\,\frac{\sin\Omega\tau}{\Omega}e^{-\gamma\tau}\langle\dot{\phi}_0(t)\dot{\phi}_0(t') + \dot{\phi}_0(t')\dot{\phi}_0(t)\rangle_{\rho_F}\right.$$

$$\left. + \Delta\int_0^t dt'\,\cos\Omega\tau e^{-\gamma\tau}\langle\dot{\phi}_0(t)\dot{\phi}_0(t') + \dot{\phi}_0(t')\dot{\phi}_0(t)\rangle_{\rho_F}\right] . \tag{4.71}$$

The correlation function for the quantum noise for the scalar field ϕ_0 which is in thermal equilibrium at a temperature $T = \beta^{-1}$ is given by

$$\langle\dot{\phi}_0(t)\dot{\phi}_0(t') + \dot{\phi}_0(t')\dot{\phi}_0(t)\rangle_{\rho_F} = \frac{2}{\pi}\int_0^\Gamma d\omega\,\omega\coth\frac{\beta\omega}{2}\cos\omega\tau , \tag{4.72}$$

where we have introduced a cut-off Γ. Now $D(t)$ can be explicitly evaluated for the field ϕ_0. It is given by

$$D(t) = -\Delta\epsilon^2\rho(k,\Delta)\left[\frac{k-\gamma\Delta}{\Omega\pi}\int_0^\Gamma d\omega\,\omega\coth\frac{\beta\omega}{2}\left(\int_0^t d\tau\,\cos\omega\tau\sin\Omega\tau e^{-\gamma\tau}\right)\right.$$

$$\left. + \frac{\Delta}{\pi}\int_0^\Gamma d\omega\,\omega\coth\frac{\beta\omega}{2}\left(\int_0^t d\tau\,\cos\omega\tau\cos\Omega\tau e^{-\gamma\tau}\right)\right] . \tag{4.73}$$

We now define the following functions:

$$f(t,\Gamma,\beta) = \frac{1}{\Omega\pi}\int_0^\Gamma d\omega\,\omega\coth\frac{\beta\omega}{2}\left[\int_0^t d\tau\,\cos\omega\tau\sin\Omega\tau e^{-\gamma\tau}\right] , \tag{4.74a}$$

$$g(t,\Gamma,\beta) = \frac{1}{\pi}\int_0^\Gamma d\omega\,\omega\coth\frac{\beta\omega}{2}\left[\int_0^t d\tau\,\cos\omega\tau\cos\Omega\tau e^{-\gamma\tau}\right] , \tag{4.74b}$$

$$h(t, \Gamma, \beta) = g - \gamma f . \tag{4.74c}$$

Using the above definitions, Eq. (4.73) becomes

$$D(t) = -\Delta \epsilon^2 [kf + \Delta h] \rho(k, \Delta) = -4\gamma \Delta [\Delta h + kf] \rho(k, \Delta) . \tag{4.75}$$

Putting this in Eq. (4.55) gives us the final form for the evolution of the reduced density matrix:

$$\dot{\rho} = \left[k \frac{\partial}{\partial \Delta} - \Delta \Omega_0^2 \frac{\partial}{\partial k} - 2\gamma \Delta \frac{\partial}{\partial \Delta} - 4\gamma \Delta^2 h(t, \Gamma, \beta) - 4\gamma \Delta k f(t, \Gamma, \beta) \right] \rho(k, \Delta) . \tag{4.76}$$

The time-dependent functions f, g, h determine the non-unitary evolution of the density matrix. To study the properties of this master equation, we transform it back to the (q, q') representation using the following relations:

$$\Delta = q - q' , \quad k = i \left[\frac{\partial}{\partial q} + \frac{\partial}{\partial q'} \right] , \tag{4.77a}$$

$$\frac{\partial}{\partial k} = -i(q + q') , \quad \frac{\partial}{\partial \Delta} = \frac{\partial}{\partial q} - \frac{\partial}{\partial q} . \tag{4.77b}$$

This results in

$$\dot{\rho}(x, x', t) = [i(\frac{\partial^2}{\partial q^2} - \frac{\partial^2}{\partial q'^2} + \Omega_0^2(q^2 - q'^2)) - 2\gamma(q - q')(\frac{\partial}{\partial q} - \frac{\partial}{\partial q'}) - 4\gamma(q - q')^2 h)]\rho$$

$$- 4i\gamma(q - q')(\frac{\partial}{\partial q} + \frac{\partial}{\partial q'})f\rho . \tag{4.78}$$

Note that we have obtained the signs of the Ω_0^2 term and the γh term as opposite to those in the paper. The first three terms in this equation denote unitary time evolution. The rest of them arise due to dissipation as well as decoherence.

We can transform the above equation to find the equation governing the evolution of the Wigner function of the system. It turns out to be [13]

$$\dot{W}(x, p) = (-\frac{\partial}{\partial q}p + \Omega_0^2 \frac{\partial}{\partial p}q + 2\gamma \frac{\partial}{\partial p}p + 4\gamma h \frac{\partial^2}{\partial p^2} - 4\gamma f \frac{\partial}{\partial q}\frac{\partial}{\partial p})W(x, p) . \tag{4.79}$$

In the subsequent sections, we study the behavior of this master equation for various systems to study its implications. We have assumed the coefficients h, f, g to be constants in the following study as these coefficients become constant after the initial transient regime [13].

4.4 The evolution of a position cat state

Position cat state is just a superposition of two Gaussians in position space whose initial wave function is given by [14]

$$\Psi_{pos}(x, t = 0) = exp[-\frac{(x - \frac{\Delta x}{2})^2}{4\delta^2}] + exp[-\frac{(x + \frac{\Delta x}{2})^2)^2}{4\delta^2}] \,, \tag{4.80}$$

where δ is the width of each of the Gaussians, Δx is the separation between them and we assume $\Delta x > \delta$.
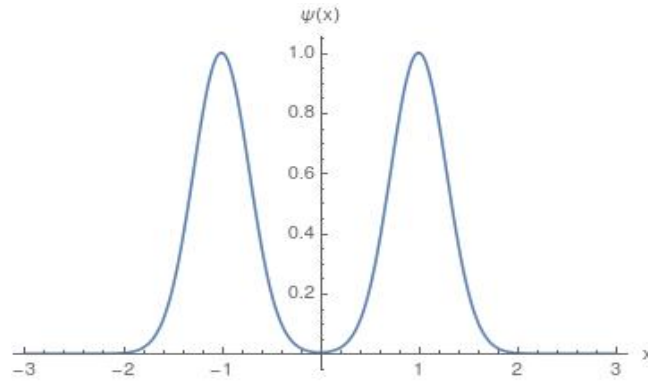

Figure 4.1: Initial state for the cat state given by Eq. (4.80) with $\Delta x = 2, \delta = 0.2$

Evolution of density matrix for the decoherence term :

The initial density matrix associated with the position cat state is,

$$\rho(x, x', 0) = \left(e^{-\frac{x - \frac{\Delta x}{2}}{4\delta^2}} + e^{-\frac{x + \frac{\Delta x}{2}}{4\delta^2}} \right) \left(e^{-\frac{x' - \frac{\Delta x}{2}}{4\delta^2}} + e^{-\frac{x' + \frac{\Delta x}{2}}{4\delta^2}} \right) . \tag{4.81}$$

Now we shall plot the evolution of the density matrix for the decoherence term alone with the initial state given by the above equation [14]. With only the decoherence term, we have

$$\dot{\rho}(x, x', t) = \tau_D^{-1}(x - x')^2 \rho(x, x') \,, \tag{4.82}$$

where τ_D is the decoherence timescale and from the analysis above it is given by $\tau_D^{-1} = 4\gamma h$. The figures in Fig. 4.2 show this evolution for the initial state given by Eq. (4.80) with $\Delta x = 2$, $\delta = 0.2$. Notice that the off-diagonal elements of the density matrix decay exponentially with time, implying the loss of quantum coherence in the position basis.

(a) time = 0
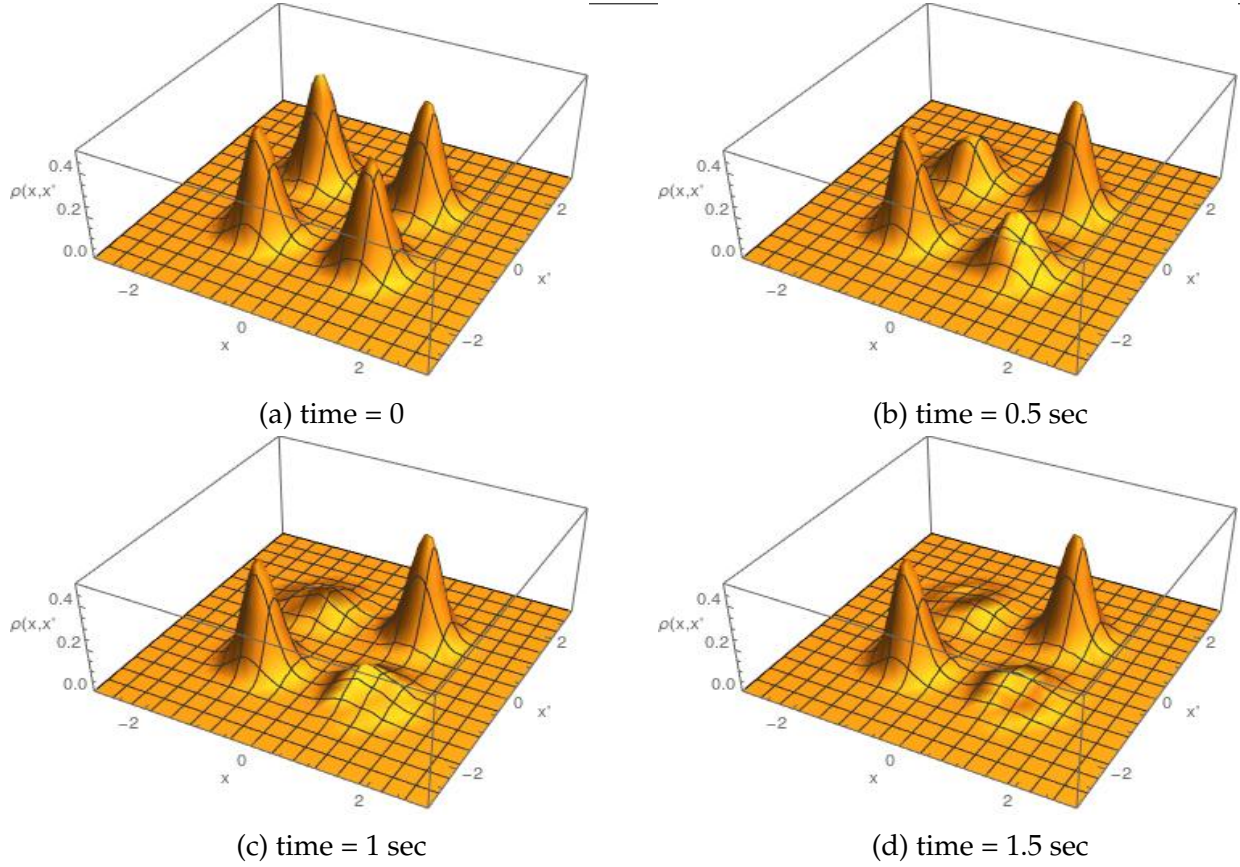
(b) time = 0.5 sec

(c) time = 1 sec

(d) time = 1.5 sec

Figure 4.2: Time evolution according to Eq. (4.82) for the cat state density matrix given by Eq. (4.81); $\tau_D = 1$ sec.

Evolution of the Wigner function of the position cat state :

We have studied the evolution of the Wigner function of the position cat state according to Eq. (4.79). The master equation for the Wigner function has been solved numerically for this purpose and the resulting evolutions in shown in Fig. 4.3. Notice that the suppression of the interference term, implying the emergence of classicality, can be clearly seen in the figures.

4.5 Evolution of the quantum harmonic oscillator

The evolution of the 9th excited state of the quantum harmonic oscillator in different limits is studied in [12] . Here we try to reproduce the results for this particular case.

(a) time = 0

(b) time = 0.05

(c) time = 0.1 s
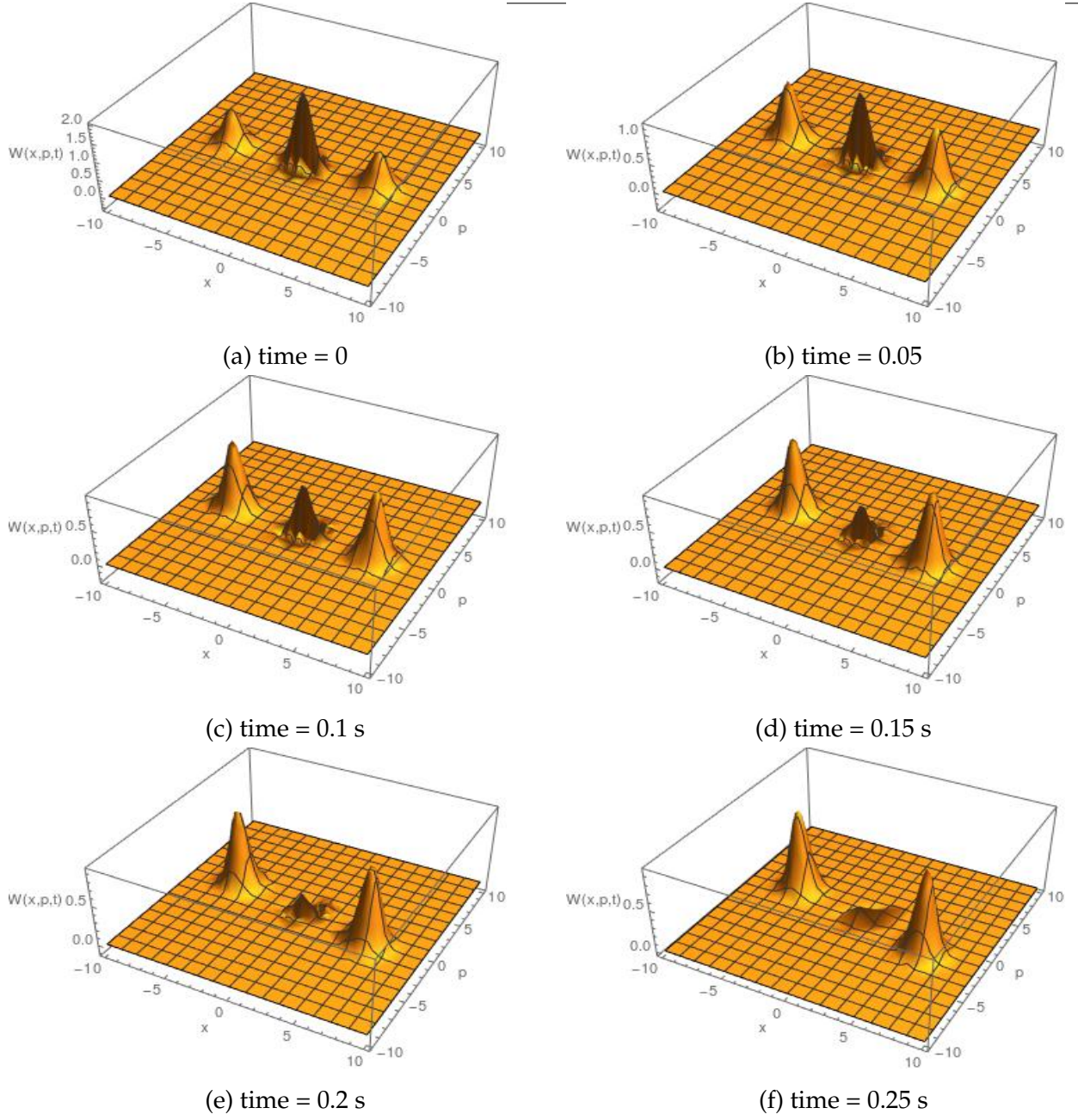
(d) time = 0.15 s

(e) time = 0.2 s

(f) time = 0.25 s

Figure 4.3: Time evolution of the Wigner function according to Eq. (4.79) with an initial position superposition (cat state) given by Eq. (4.80). $\Delta x = 6, \delta = 1, \gamma = 0.1, \Omega_0 = 1, h = 0.1, f = 0.01$.

The 9th excited state for the quantum harmonic oscillator is given by (see Fig. 4.4)

$$\Psi(x, t = 0) = Ae^{-\frac{m\omega x^2}{2\hbar}} H_9\left(\sqrt[2]{\frac{m\omega}{\hbar}}x\right), \quad (4.83)$$

where A is the normalization constant, m is the mass and ω is the angular frequency of the
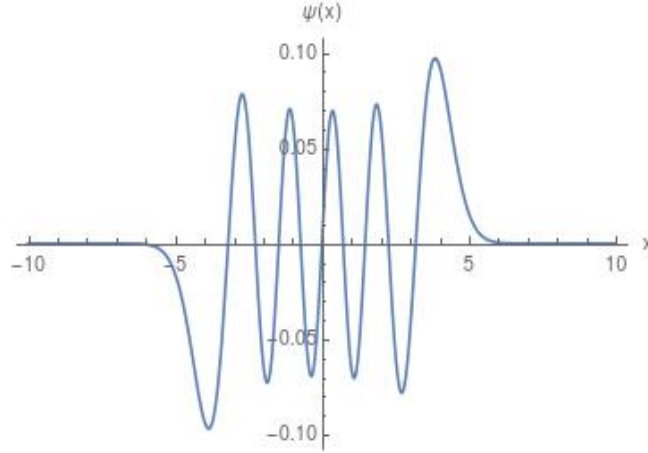
oscillator .

Figure 4.4: Wave function associated with the 9th excited state of the harmonic oscillator, given by Eq. (4.83). The parameters have been set to unity, i.e., $m = \omega = \hbar = 1$

Evolution of density matrix for the 9th excited state of quantum harmonic oscillator :

The evolution of the density matrix for the 9th excited state of the quantum harmonic oscillato due only to decoherence component is plotted in Fig. 4.5. Notice again the decaying of the off-diagonal elements of the density matrix denoting the loss of coherence.

Evolution of the Wigner function for the 9th excited state :

The evolution of the Wigner function according to Eq. (4.79) for the initial state given by Eq. (4.83) is shown in Fig. 4.6. The solution was obtained by numerically solving Eq. (4.79) for $\gamma = 1$, $\Omega_0 = 1$, $h = 1$ and $f = 0.01$. Notice how the initial symmetry between position and momentum is broken due the form of the environmental coupling of the forcing field ϕ with x. Also notice the way superpositions have died out with the passage of time.
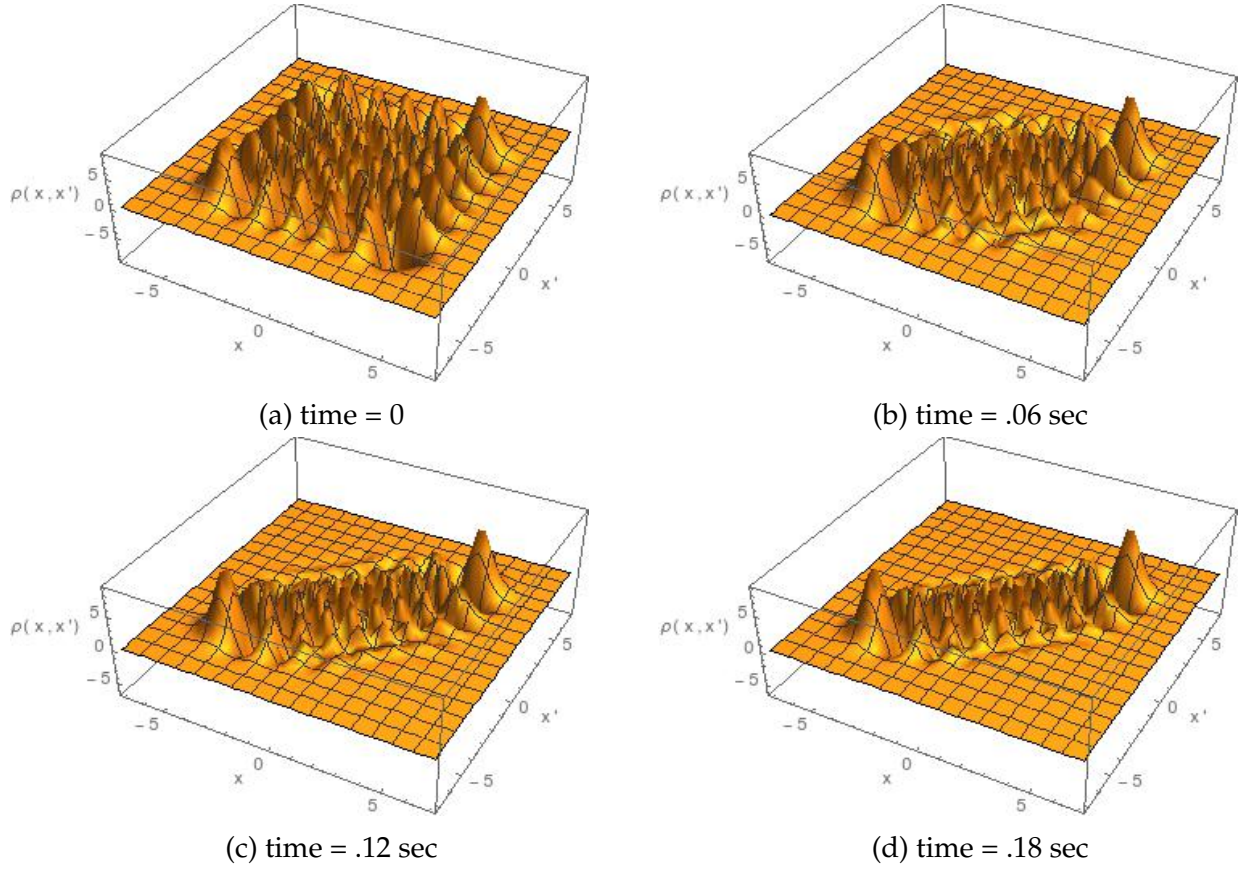
(a) time = 0

(b) time = .06 sec

(c) time = .12 sec

(d) time = .18 sec

Figure 4.5: Time evolution according to Eq. (4.82) for the density matrix of the 9th excited state of the quantum harmonic oscillator given by Eq. (4.83). τ_D was chosen to be unity while plotting these figures.

(a) time = 0

(b) time = 0.15 sec

(c) time = 0.3 sec
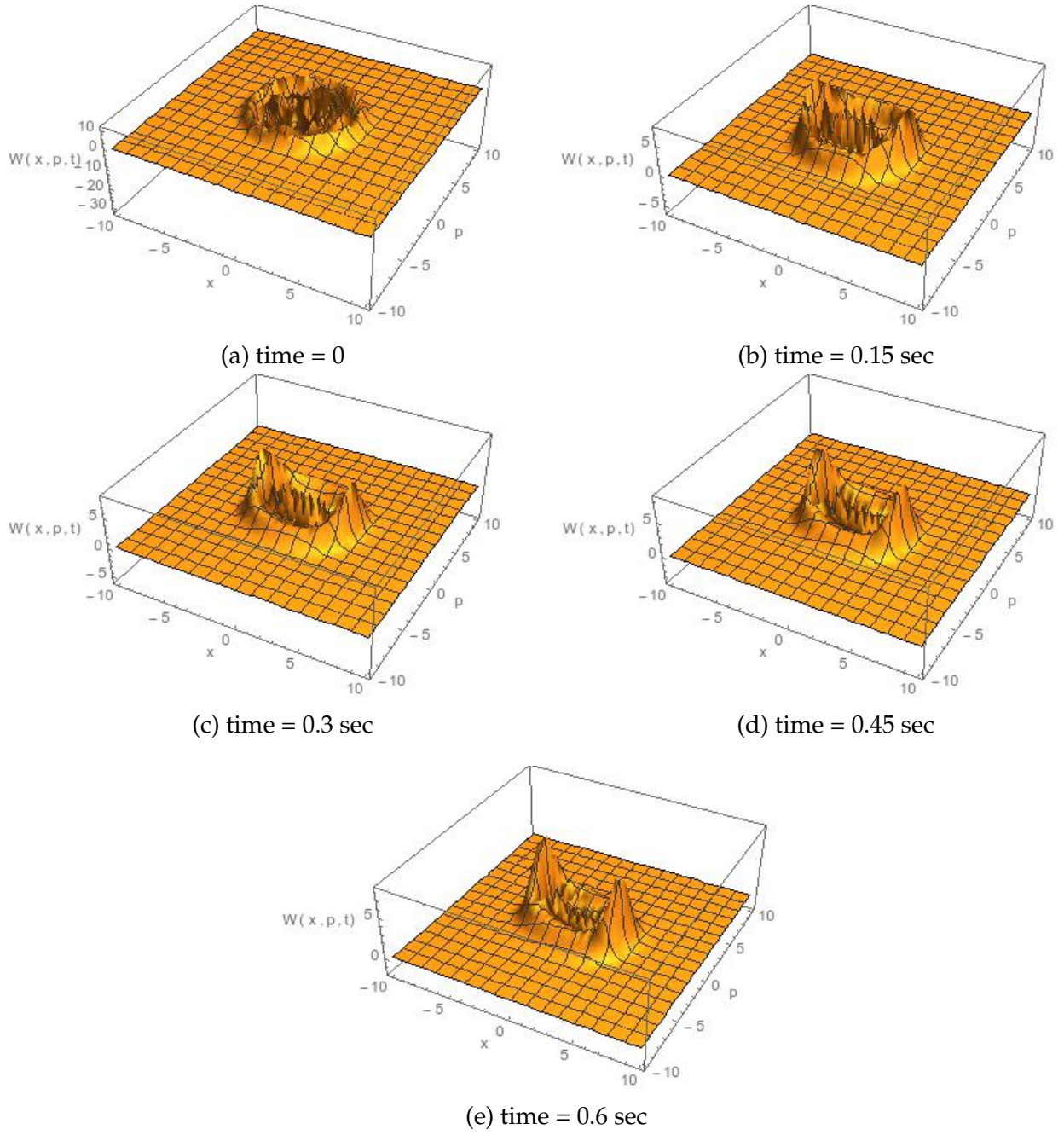
(d) time = 0.45 sec

(e) time = 0.6 sec

Figure 4.6: Time evolution of the Wigner function according to Eq. (4.79) for the 9th excited state of the quantum harmonic oscillator is plotted here. The solutions were obtained by numerically solving Eq. (4.79) for $\gamma = 1$, $\Omega_0 = 1$, $h = 1$ and $f = 0.01$.

Chapter 5

Summary

In this work, we have shown how systems lose their quantum nature by virtue of their inter-action with the environment. We began our work by discussing some of the key features of quantum mechanics that give it a distinctive color in the mundane world of human common sense and makes it stand apart. Afterwards, we show how those features slowly fade away in the abyss of the macroscopical domain. We set out to seek what causes this transition and at our first stop meet some experiments. These experiments told us that the reason behind this transition isn't just our unfortunate inability of "see"-ing these exotic features, which become too minuscule as we enter the "big" world of basketballs and bananas. The story goes down the rabbit hole. They whispered into our ears stories of the omnipresence of na-ture, of the environment, which becomes unavoidable as we climb up the ladder of size and sang to us how this mingling (entanglement) of the environment with buckyballs (system) leads to a transfer of quantum features from the system to the global level. Motivated by their chants, we first armed ourselves with certain tools such as density matrices and Wigner functions, which were necessary to study systems that are not selfishly closed. We saw some examples of these constructs for various systems and understood what they imply. Then we finally delved into the study of open quantum systems, to find that depending upon the way a system interacts with the environment, certain system quantum states are preferred over others. The environmental interaction leads to the emergence of a set of "pointer states" which get least entangled with the environment and a superposition of these states loses its quantum coherence quite rapidly. Next we focused our attention on the system alone and tried to construct equations that denote the evolution of the system with minimal input from the environment. These "master equations", specifically the Born-Markov master equation,

derived under certain approximate assumptions, sometimes lead to the violation of positivity of density matrices, a very undesirable feature, but the ones which could be written in a Lindblad form were free of this sin. The master equations made our lives simpler by a great deal as we didn't have to take care of the environmental degrees of freedom, which were often too large to take care of anyways, and they let us construct simplistic models of the system-environment interaction to derive observable effects thereof. Finally, in the last chapter, we took up a specific model of system-environment interaction, known as the quantum Brownian motion, and derived the master equation along with its solutions for the particular case. We finally ended our work by studying the evolution of different initial states under this master equation. We plotted these numerically obtained solutions to find that indeed the superposition of certain states lose their quantum nature in the course of time, giving a concrete appeal to the theory we had developed up to that point and bringing our quest to a temporary end.

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