

Introduction:

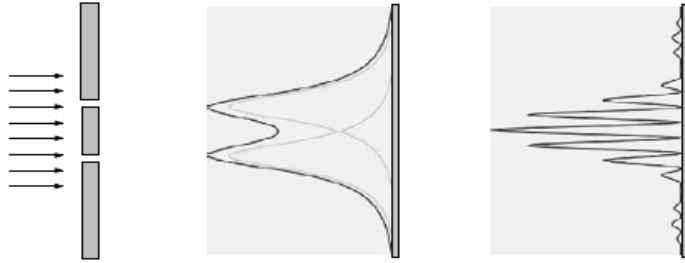
A cornerstone of modern physics, quantum mechanics governs the behavior of particles and their interactions at the microscope scale. It uncovers phenomenon such as superposition and entanglement whereby particles exhibit wave-like nature and seem to influence each other non-locally. Yet, as we shift our focus to the macroscopic scale, this quantum nature appears to fade, giving way to the familiar classical laws laid down by classical mechanics. At the heart of this quantum-to-classical transition is the concept known as decoherence. Decoherence refers to the gradual loss of quantum coherence and the emergence of classical behavior in large systems. Not only does it explain why we don't see quantum effects on macroscopic scales, it holds immense significance in our pursuit of harnessing the power of quantum principles for practical applications such as quantum cryptography and quantum communication. For instance, breaking RSA codes and developing efficient search algorithms are just a couple of areas where quantum computing holds promise. Moreover, investigating decoherence provides an opportunity to delve deeper into the foundations of quantum mechanics itself. By unraveling the intricate mechanisms behind decoherence, our understanding of quantum measurement and the controversial collapse postulate can be challenged and new insights can be gained that resolve the fundamental time-asymmetry that interaction via measurement introduces into quantum systems.

How the act of measurement changes the state of the system:

In the double slit experiment, there exists two limiting regimes, each governed by the act of measurement:

1. The “wave” scenario (illustrated on the right of Figure below). In that case, the general wavefunction is that of a two-level system with the wavefunction being in a superposition state $\Psi_s = \frac{1}{\sqrt{2}} [\Psi_1(x) + \Psi_2(x)]$. If we refrain from measuring through which slit each particle has passed, the particle density observed at the level of the detecting screen corresponds to an interference pattern given by $p(x) = |\Psi_s|^2 = \frac{1}{2} |\Psi_1(x) + \Psi_2(x)|^2$ where $p(x)$ corresponds to the probability density function. That is, if we refrain from measurement, the probability density corresponds to a quantum-mechanic superposition of the partial waves $\Psi_1(x)$ and $\Psi_2(x)$ representing passage through slit 1 and 2 respectively.
2. The “particle” scenario (shown in the center of Figure below). If we place a detector at one of the slits to find out whether the particle has passed through this slit, the interference pattern disappears. In that case, by invoking postulate 5 II) of Quantum Mechanics, we say that the *wavefunction* has collapsed, say, for example to $\Psi_1(x)$ such that we have $\Psi_s \rightarrow \Psi_1$. Now the density pattern on the distant screen is simply equal to a classical addition of the pattern created by all particles that have traversed slit 1 (that is,

the pattern that would be obtained if slit 2 was covered) and the pattern created by all particles that have passed through slit 2: $p(x) = |\Psi_1(x)|^2$



The standard explanation of the second case is given by the Collapse Postulate of Quantum Mechanics. According to Quantum Mechanics, the state of the particle at the level of the slits is given by the superposition $\Psi(x) = \frac{1}{\sqrt{2}} (\Psi_1(x) + \Psi_2(x))$ of the partial waves $\Psi_1(x)$ and $\Psi_2(x)$. This superposition is spatially spread out over the region encompassing the two slits. If we now measure the position of the particle at one of the slits and indeed find the particle to be present at this slit, we localize $\Psi(x)$ to the corresponding spatial region. That is, since $\Psi_1(x)$ and $\Psi_2(x)$ have negligible overlap at the level of the slits, we may say that, using the standard collapse postulate of quantum mechanics, the measurement has collapsed the superposition $\Psi(x)$ onto either one of the component states $\Psi_1(x)$ or $\Psi_2(x)$. Thus we can no longer obtain interference between these partial waves, and hence the interference pattern on the distant screen disappears.

Hence, whenever we try to obtain which-path (“Welcher-Weg”) information about the particle in order to see which of the two slits the particle has traversed—i.e., whenever we attempt to make sense of the quantum mechanical superposition of the two paths that would seem to describe a counterintuitive simultaneous passage through both slits—it seems that we cannot help but destroy the ability of the particle to exhibit the quantum property of (spatial) interference.

Density matrix formulation:

In this subsection, we are going to build towards a wonderful, exciting development in the foundation of Quantum Mechanics. For a double slit-experiment, Wojciech Hubert Zurek and William Wootters established that we can actually retain parts of the interference pattern by gathering only some which-path information, e.g, by performing an imprecise measurement of which slit the particle has traversed. To discuss the features which allow us to do this, the description in terms of wave-function collapse will no longer be suitable. By postulate, the collapse of the wavefunction is a discontinuous, irreversible process and therefore cannot account for smooth, reversible changes in the amount of which-path information and the degree of interference. Instead, we shall pursue an entirely new formalism in terms of density matrices.

Just like before, let us denote the quantum states of the particle corresponding to passage through slit 1 and 2 by $|\Psi_1\rangle$ and $|\Psi_2\rangle$ respectively. As before, we place a detector at each of the two slits, with both detectors initially in the “ready” state. We can prepare our particle, in say, the state $|\Psi_1\rangle$ by covering slit 2, and placing the particle source directly behind slit 1 such that the particle will be guaranteed to pass through this slit. Consequently, the detector associated with slit 1 will trigger, while the detector at slit 2 will remain in the untriggered “ready” state.

We denote the joint “ready” state of the (composite) detector by $|\text{ready}\rangle$ and the quantum state of this detector system after preparation of the state $|\Psi_1\rangle$ by $|1\rangle$, indicating the passage of the particle through slit 1. Thus, in this case, the evolution of the composite particle-detector system will be of the form:

$$|\Psi_1\rangle |\text{ready}\rangle \rightarrow |\Psi_1\rangle |1\rangle \rightarrow (1.1)$$

Repeating the above argument with the role of the slits reversed yields the evolution:

$$|\Psi_2\rangle |\text{ready}\rangle \rightarrow |\Psi_2\rangle |2\rangle \rightarrow (1.2)$$

On the other hand, if both slits are open, the particle must be described by a superposition by $|\Psi\rangle = \frac{1}{\sqrt{2}}(|\Psi_1\rangle + |\Psi_2\rangle)$ of the two components $|\Psi_1\rangle$ and $|\Psi_2\rangle$. Therefore, we obtain a dynamical evolution of the von Neumann type, leading to an entangled composite particle-detector state,

$$\frac{1}{\sqrt{2}}(|\Psi_1\rangle + |\Psi_2\rangle)|\text{ready}\rangle \rightarrow \frac{1}{\sqrt{2}}(|\Psi_1\rangle|1\rangle + |\Psi_2\rangle|2\rangle) \rightarrow (1.3)$$

Expressing (1.3) in terms of density matrix, we have:

$$\begin{aligned} \hat{p} &= \frac{1}{2}[(|\Psi_1\rangle|1\rangle + |\Psi_2\rangle|2\rangle)(\langle\Psi_1|\langle 1| + \langle\Psi_2|\langle 2|)] \\ \hat{p} &= \frac{1}{2}(|\Psi_1\rangle\langle\Psi_1||1\rangle\langle 1| + |\Psi_1\rangle\langle\Psi_2||1\rangle\langle 2| + |\Psi_2\rangle\langle\Psi_1||2\rangle\langle 1| + |\Psi_2\rangle\langle\Psi_2||2\rangle\langle 2|) \end{aligned}$$

Where $|1\rangle\langle 1| = |2\rangle\langle 2| = 1$ such that:

$$\hat{p} = \frac{1}{2}(|\Psi_1\rangle\langle\Psi_1| + |\Psi_1\rangle\langle\Psi_2||1\rangle\langle 2| + |\Psi_2\rangle\langle\Psi_1||2\rangle\langle 1| + |\Psi_2\rangle\langle\Psi_2|) \rightarrow (1.4)$$

The Probability density can then be written using the Born’s Rule as:

$$\begin{aligned} p(x) &= \left(\frac{1}{\sqrt{2}}(|\Psi_1\rangle|1\rangle + |\Psi_2\rangle|2\rangle)\right) \left(\frac{1}{\sqrt{2}}(\langle\Psi_1|\langle 1| + \langle\Psi_2|\langle 2|)\right) \\ p(x) &= \frac{1}{2}|\Psi_1(x)|^2 + \frac{1}{2}\langle\Psi_2|\Psi_1\rangle\langle 2|1\rangle + \frac{1}{2}\langle\Psi_1|\Psi_2\rangle\langle 1|2\rangle + \frac{1}{2}|\Psi_2(x)|^2 \end{aligned}$$

By Symmetry of inner product, that is, $\langle u, v \rangle = \langle v, u \rangle$, we have:

$$p(x) = \frac{1}{2}|\Psi_1(x)|^2 + \frac{1}{2}|\Psi_2(x)|^2 + \langle\Psi_1|\Psi_2\rangle\langle 2|1\rangle \rightarrow (1.5)$$

The last term describes the interference pattern, and we see that the visibility of the interference pattern is quantified by the overlap $\langle 2|1 \rangle$. In particular, the limiting case of distinguishability of the detector states $|1\rangle$ and $|2\rangle$, $\langle 2|1 \rangle = 0$ corresponds to the “particle” regime,

$$p(x) = \frac{1}{2} |\Psi_1(x)|^2 + \frac{1}{2} |\Psi_2(x)|^2 \rightarrow (1.6)$$

Conversely, if $|1\rangle$ and $|2\rangle$ are unable to resolve the path of the particle $\langle 2|1 \rangle = 1$ disregarding phase factors, the wave-scenario of full interference pattern applies:

$$p(x) = \frac{1}{2} |\Psi_1(x)|^2 + \frac{1}{2} |\Psi_2(x)|^2 + \langle \Psi_1 | \Psi_2 \rangle \rightarrow (1.7)$$

Looking beyond Copenhagen Interpretation:

Using equation (1.6), we are in position to formulate a physical model of double slit experiment that is much more causal and continuous than Copenhagen interpretation which introduces the controversial collapse postulate

The situation in which the detector obtains some but not full which-path information is formally represented by an overlap of the two detector states $|1\rangle$ and $|2\rangle$ that is nonzero but less than one. From equation (1.2), we see that we will be able to observe an interference pattern, but the pattern will decay progressively as the overlap $\langle 2|1 \rangle$ *decreases* and thus the amount of which path information obtained by the detector *increases*.

Thus we have shown that it is indeed possible to simultaneously observe an interference pattern and obtain some information about the path of the particle through the slits, provided this information remains incomplete. As soon as the information acquired by the detector is sufficient to enable us to infer with certainty which path the particle has taken, the interference pattern disappears.

Simple Model of Decoherence:

Suppose you have the conventional Stern-Gerlach Setup where now the electrons passing through the device are now coming into interactions with photons of two different orientations. In general, we have a model consisting of a central quantum two-level system S linearly coupled to an environment \mathcal{E} composed of a collection of N other quantum two-level systems.

In the following, let us denote the two basis states of our main system S by $|0\rangle$ and $|1\rangle$, while we shall use $\{ |\uparrow\rangle_i, |\downarrow\rangle_i \}$ where $i = 1 \dots N$, to represent the basis states of the N two-level systems of the environment.

We describe the total system–environment combination by the Hilbert space:

$$\mathcal{H} = \mathcal{H}_S \otimes \mathcal{H}_{\varepsilon_1} \otimes \mathcal{H}_{\varepsilon_2} \otimes \dots \otimes \mathcal{H}_{\varepsilon_N} \rightarrow (2.1)$$

Consider now the form that the Hamiltonian would take. Since we are dealing with spin $\frac{1}{2}$ particle, then we can use Pauli Matrices to represent their Hamiltonian. In particular, we align the experiment along the z-direction to obtain the following Hamiltonian:

$$\mathcal{H}_{int} = \frac{1}{2} \widehat{\sigma}_z \otimes \sum_{i=1}^N g_i \widehat{\sigma}_z^{(i)} \rightarrow (2.2)$$

Where the coupling strength is given by the constants g_i , $i = 1 \dots N$. From equation (2.2), we see that the environment monitors the observable $\widehat{\sigma}_z$, i.e., the z-spin component of the system. Thus we conclude without any calculation that the eigenbasis $\{ |0\rangle, |1\rangle \}$ of $\widehat{\sigma}_z$ to emerge as the dynamically selected preferred basis of the system. Superposition states of $|0\rangle$ and $|1\rangle$ will be prone to decoherence, whereas $|0\rangle$ and $|1\rangle$ will represent the dynamically robust states of the system.

From equation (2.2), we also observe that, since the Hamiltonian commutes with the Pauli operator $\widehat{\sigma}_z$ of the system, the populations of the system are conserved quantities under the action of this Hamiltonian. There is no exchange of energy between the system and the environment, and therefore the interaction with the environment can influence only the degree of coherence present in the system.

The eigenstate of the total Hamiltonian \mathcal{H}_{int} are of the form $|0\rangle|n\rangle$ and $|1\rangle|n\rangle$ where,

$$|n\rangle = |\uparrow\rangle_1, |\uparrow\rangle_2, \dots, |\uparrow\rangle_N \rightarrow (2.3)$$

$$\text{Where } 0 \leq n \leq 2^N - 1.$$

Since these states form a basis of the composite system $S\varepsilon$ can be expanded as:

$$|\Psi\rangle = \sum_{n=0}^{2^N-1} c_n |0\rangle|n\rangle + d_n |1\rangle|n\rangle \rightarrow (2.4)$$

Time-Evolution of the Decoherence Model:

Let us now assume that $t = 0$, before the interaction between S and ε is turned on, the system and the environment are completely uncorrelated, i.e, that the initial state $|\Psi(0)\rangle$ of $S\varepsilon$ factorizes into a product state of the form:

$$|\Psi\rangle = (a |0\rangle + b |1\rangle) \sum_{n=0}^{2^N-1} c_n |n\rangle \rightarrow (2.5)$$

Then the time evolution of the *state* $S\varepsilon$ generated by the action of the Hamiltonian is given by:

$$|\Psi(t)\rangle = e^{-i\hat{H}t} |\Psi(0)\rangle$$

$$|\Psi(t)\rangle = e^{-i\hat{H}t} \left((a|0\rangle + b|1\rangle) \sum_{n=0}^{2^N-1} c_n |n\rangle \right) \rightarrow (2.55)$$

$$|\Psi(t)\rangle = a|0\rangle|\varepsilon_0(t)\rangle + b|1\rangle|\varepsilon_1(t)\rangle \rightarrow (2.6)$$

Where,

$$|\varepsilon_0(t)\rangle = \sum_{n=0}^{2^N-1} c_n e^{\frac{i\varepsilon_n t}{2}} |n\rangle \rightarrow (2.61)$$

$$|\varepsilon_1(t)\rangle = \sum_{n=0}^{2^N-1} c_n e^{\frac{i\varepsilon_n t}{2}} |n\rangle \rightarrow (2.62)$$

Note that the logic from going from line (2.55) to (2.6) is similar to the argument we carried out in exposition 5) Stern Gerlach Revisited. Essentially, the Hamiltonian acts on states of the form $|\uparrow\rangle$ and $|\downarrow\rangle$ to give the associated eigenvalues with it. Essentially then just like in that exposition, (2.61) and (2.62) acts as pointer states that essentially yields our overlap integral:

$$r(t) \equiv \langle \varepsilon_1(t) | \varepsilon_0(t) \rangle = \sum_{n=0}^{2^N-1} |c_n|^2 e^{i\varepsilon_n t} \rightarrow (2.7)$$

Evaluating the Density Matrix:

We are now ready to evaluate the density matrix of the system. We have:

$$|\Psi\rangle\langle\Psi| = [a|0\rangle|\varepsilon_0(t)\rangle + b|1\rangle|\varepsilon_1(t)\rangle] [\langle 0| \langle \varepsilon_0(t)| a^* + \langle 1| \langle \varepsilon_1(t)| b^*]$$

$$\begin{aligned} |\Psi\rangle\langle\Psi| &= a^2 |0\rangle\langle 0| \langle \varepsilon_0(t) | \varepsilon_0(t) \rangle + ab^* |0\rangle\langle 1| \langle \varepsilon_0(t) | \varepsilon_1(t) \rangle \\ &\quad + ba^* |1\rangle\langle 0| \langle \varepsilon_1(t) | \varepsilon_0(t) \rangle + b^2 |1\rangle\langle 1| \langle \varepsilon_1(t) | \varepsilon_1(t) \rangle \end{aligned}$$

Where $\langle \varepsilon_0(t) | \varepsilon_0(t) \rangle = \langle \varepsilon_1(t) | \varepsilon_1(t) \rangle = 1$ such that:

$$|\Psi\rangle\langle\Psi| = a^2 |0\rangle\langle 0| + ab^* |0\rangle\langle 1| r(t) + ba^* |1\rangle\langle 0| r^*(t) + b^2 |1\rangle\langle 1|$$

$$\hat{\rho} = a^2 |0\rangle\langle 0| + ab^* |0\rangle\langle 1| r(t) + ba^* |1\rangle\langle 0| r^*(t) + b^2 |1\rangle\langle 1| \rightarrow (2.8)$$

The Time-evolution of the Decoherence Factor:

The interesting question, of course, considers the time-evolution of the decoherence factor $r(t)$. Consider the equation:

$$r(t) \equiv \sum_{n=0}^{2^N-1} |c_n|^2 e^{i\varepsilon_n t} \rightarrow (2.9)$$

From the equation, we see that $r(t)$ corresponds to the addition of 2^N vectors of length $|c_n|^2$ rotating in the complex with different frequencies proportional to ε_n . Since $\sum_{n=0}^{2^N-1} |c_n|^2 = 1$, the average step length $\langle |c|^2 \rangle$ will be equal to 2^{-N} . For example, if $N = 1$, then we have two vectors

and in order for them to equal 1, we have: $\frac{1}{2} + \frac{1}{2} = 1$. Similarly, if $N = 2$, then we have four vectors and in order for them to equal 1, we would have $\frac{1}{4} + \frac{1}{4} + \frac{1}{4} + \frac{1}{4} = 1$ and so on... This implies that the length of the complex vector $r(t)$ will scale as:

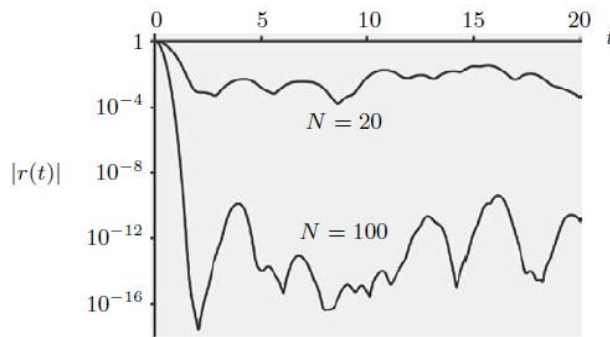
$$\langle |r(t)|^2 \rangle \propto \langle |c|^2 \rangle = 2^{-N} \rightarrow (2.10)$$

This shows that the degree of suppression of coherence in the $\{|0\rangle, |1\rangle\}$ scales exponentially with the size N of the environment. Furthermore, Zurek and Co were able to show that for sufficiently large N and a large class of distributions of the coupling, $r(t)$ follows an approximate Gaussian decay with time:

$$r(t) \approx e^{-\tau^2 t^2} \rightarrow (2.11)$$

The Recurrence Time :

However, it is important to realize that, as long as the number of environmental spins (and thus the number of degrees of freedom in the environment) is finite, there always exists a characteristic recurrence time τ_{rec} for which the decoherence factor in equation (7) will return to its initial value of one. This is simply a consequence of the fact that equation (7) is a sum of functions that are periodic in time. Any such sum of periodic functions must in turn be periodic, too. The value of the recurrence time depends on the initial state of the environment and the distribution of the couplings g_i . The characteristic recurrence time τ_{rec} is typically extremely long and of the Poincare's type with $\tau_{rec} \propto N!$. For macroscopic environments of realistic but finite sizes, τ_{rec} can exceed the lifetime of the universe, as first pointed out by Zurek [9]. Thus the loss of coherence from the system is typically irreversible for all practical purposes not only because of our practical inability to control and observe the environment, but also because the timescale for the recurrence of coherence is astronomically large in virtually all physically realistic situations.



The figure shows the evolution of the absolute value of the decoherence factor $r(t)$ describing the time dependence of inference terms in a central spin system interacting with a collection of N static environmental spins for two different values $N = 20$ and $N = 100$. The initial state of each environmental spin was assumed to be completely random, with the environmental spin completely uncorrelated with each other and with the system. The couplings were chosen randomly from the interval $[0,1]$

Master Equation formulation:

Master equations directly and conveniently yield the time evolution of the reduced density matrix $\hat{\rho}_S(t)$ for the open quantum system S interacting with an environment E. They relieve us from the need of having to first determine the dynamics of the total system–environment combination and to then trace out the degrees of freedom of the environment. The master-equation approach is motivated by two issues. First, we are usually not interested in the dynamics of the environment or of the global system–environment combination. All we really care about is the influence of the environment on our system of interest. Second, it is often impossible to analytically determine the time evolution of the density matrix. In such cases, one can use approximation schemes that lead to master equations for the approximate evolution of the reduced density matrix

In contrast with the dynamics of the density matrix of a closed system, the evolution equation for the reduced density matrix will be nonunitary

Refresher: Why is Unitary Evolution important?

Firstly, let's try to understand why this is a big deal. Unitary time evolution is the specific type of time evolution where probability is conserved. In quantum mechanics, one typically deals with unitary time evolution. Suppose you have a state (at time $t = 0$) given by $|\alpha\rangle$. To find the state at a later time $t = T$ given by $|\alpha(T)\rangle$, we apply the unitary time evolution operator U :

$$U|\alpha\rangle = |\alpha(T)\rangle$$

Where $U = e^{-iHt}$ and H = Hamiltonian of the system, which is Hermitian. Conservation of probability mathematically means:

$$\langle \alpha | \alpha \rangle = \langle \alpha(T) | \alpha(T) \rangle$$

Physically, it means that the probability of existence of the quantum system, described initially by the state $|\alpha\rangle$ and later by $|\alpha(T)\rangle$, does *not* change with time. The quantum system exists at $t=0$ with probability =1, and also at $t=T$ with probability = 1. The state evolves in time from $t=0$ to $t=T$, but no information about the quantum system leaks out during this time interval. The system that existed at $t=0$ continues to exist in its totality later at $t=T$. This is physically meaningful to demand from a theory, because information about a state should not get lost during evolution. Sure, the information might get tangled up as time goes on, but *all of it* should still be there, in principle. For example, if you burn a book on coal, information inside the book is lost for all practical purposes. But, all information *still* exists, *in principle*, encoded in the correlations between coal and ash particles.

Introducing Non-Unitary Time-evolution:

Sometimes, it is easier/useful to explain certain phenomena by abandoning unitary time evolution, for instance, in unstable particles or radioactive decay. There, as time goes on, the mother state decays into daughter states. If you observe *only* the mother state *subsystem*, it does *not* undergo unitary time evolution because it loses information about its state with the passage of time. The information is lost to the daughter state subsystems. Probability (of the mother state existing) is not conserved; it decreases (exponentially) with time. If you look at the *full* system, as whole, evolution is unitary, as expected. But in radioactivity, we often just need to know how the mother state *subsystem* disintegrates.

Lets now introduce non-unitary time-evolution in context of our situation. Consider a statistical mixture of pure systems i.e. assume that there is an ensemble of systems so that a fraction p_1 is in state $|1\rangle$, p_2 are in state $|2\rangle$ and so on. Then the entire statistical ensemble can be described by a so-called density matrix $\rho = \sum_i |i\rangle\langle i|$. We can consider the evolution of this density operator, which is often written as the so-called Liouville equation $\frac{d\rho}{dt} = \mathcal{L}\rho$. Here \mathcal{L} is the “Liouvillian” an operator that transitions ρ in time much like U transitions the pure state in time for a pure state.

If the dynamics is governed by a Hamiltonian, then the Liouvillian (the “propagator” of the state) is simply its commutation relation with the state $\mathcal{L} = -i / \hbar (\mathbf{H}\rho - \rho\mathbf{H})$. This corresponds to standard Hamiltonian evolution, and is unitary. Consider, however, looking at only a subsystem of the extended system. The state of such a subsystem can be described by a “reduced” density operator. However, even though the evolution of the extended system is unitary and follows a Hamiltonian, the evolution of the subsystem's density generally *does not* follow a Hamiltonian and is not unitary. Instead, it is often “dissipative”. For example, the subsystem might dissipate energy into the environment and cool down into a thermal state. density operator, which is really just a density operator (matrix) describing the subsystem.

There is no general simple form for the Liouvillian (the propagator) for subsystems. A relatively simple case is when the subsystem evolves in a Markovian manner, which is often the case for systems equilibrating thermally. Then the Liouvillian has a unitary term, driven by a Hamiltonian just as above, but also a correction: a non-Hamiltonian term, a term which follows a special form called “Lindblad form” rather than the commutation-with-the-state written above.

So - non unitary evolution is actually everywhere. Whenever you can't neglect the interactions with the environment, so that you e.g. equilibrate thermally with it, you have non-unitary evolution (there are a few caveats, but it's almost always true). What's difficult is getting a unitary evolution going. You have to isolate your system from the environment enough to be able to neglect thermalization etc.

The biggest difference, perhaps, between these two kinds of evolutions is that non-unitary evolution is (generically) not reversible. That's how you get thermalization. Non-unitary dynamics can also change the populations, reflecting for example a decrease in highly-energetic states as the system cools down towards its ground-state.

General Formalism:

In the “ordinary” formalism of decoherence, the reduced density matrix $\hat{p}_s(t)$ is computed via:

$$\hat{p}_s(t) = Tr_{\mathcal{E}}(\hat{p}_{s\mathcal{E}}(t)) \equiv Tr_{\mathcal{E}}(\hat{U}(t)\hat{p}_{s\mathcal{E}}(0)\hat{U}^\dagger(t)) \rightarrow (3.1)$$

Where $\hat{U}(t)$ denotes the time-evolution operator for the composite system $S\mathcal{E}$. As is evident from (1), this approach inevitably requires that we first determine the dynamics $\hat{p}_{s\mathcal{E}}(t)$ of the total system $S\mathcal{E}$ before we can arrive at the reduced description through the trace operation. As we have indicated that in the situations where system is interacting with the environment, this task is very difficult, if not impossible for most reasonably complex model systems.

By contrast, in the master-equation formalism, we instead calculate $\hat{p}_s(t)$ directly from an expression of the form:

$$\hat{p}_s(t) = \hat{V}(t)\hat{p}_s(0) \rightarrow (3.2)$$

Where the operator $\hat{V}(t)$ is so called dynamical map that generates the evolution of $\hat{p}_s(t)$. Since $\hat{V}(t)$ represents an operator that in turn acts on another operator, it is commonly referred to as a “superoperator.”. Equation (3.2) is called a master equation for $\hat{p}_s(t)$ and it represents the most general form that such a master equation may take.

If the master equation is exact, then it is obviously unitary such that (3.1) and (3.2) must be equivalent such that we have:

$$\hat{V}(t)\hat{p}_s(0) = Tr_{\mathcal{E}}\{\hat{U}(t)\hat{p}_{s\mathcal{E}}(0)\hat{U}^\dagger(t)\} \rightarrow (3.3)$$

However, the true power of master equation arises from its ability to deal with non-unitary evolution. To that extent, its capacity is fully unveiled when we impose certain assumptions about the system–environment states and dynamics. Such assumptions then allow us to determine the approximate time evolution of \hat{p}_s even when it is impossible to calculate the exact global dynamics $\hat{p}_{s\mathcal{E}}(0)$. In fact, here we shall restrict our attention to master equations (obtained from certain approximations) that can be written as first-order differential equations that are local in time, i.e., that can be expressed in the form:

$$\frac{d}{dt}\hat{p}_s(t) = \hat{\mathcal{L}}[\hat{p}_s(t)] = -i[\hat{H}'_s, \hat{p}_s(t)] + \hat{\mathcal{D}}[\hat{p}_s(t)] \rightarrow (3.4)$$

This equation is local in time in the sense that the change of \hat{p}_s at time t depends only on \hat{p}_s evaluated at t but not at any other times $t' = t$. The superoperator $\hat{\mathcal{L}}$ appearing in (3.4) acts on $\hat{p}_s(t)$ and typically depends on the initial state of the environment and the different terms in the Hamiltonian.

To convey the physical intuition behind this superoperator, $\hat{\mathcal{L}}$ has been decomposed into two parts:

1. A unitary part that is given by the usual Liouville–von Neumann commutator with the Hamiltonian \hat{H}'_S . It is important to note that this Hamiltonian is in general not identical to the unperturbed free Hamiltonian \hat{H}_S of S that would generate the evolution of S in absence of the environment, because the presence of the environment often perturbs the free Hamiltonian, leading to a renormalization of the energy levels of the system. We emphasize that this effect (often called the Lamb-shift contribution) has nothing to do with the nonunitary evolution induced by the environment but only alters the unitary part of the reduced dynamics.
2. A nonunitary part $\hat{D} [\hat{\rho}_S(t)]$ that represents decoherence (and possibly also dissipation) due to the environment. This term will be of the most interest to us in the following.

We note that, if the evolution of the system is completely unitary, we have $\hat{D} [\hat{\rho}_S(t)] = 0$, and thus (4) simply becomes:

$$\frac{d}{dt} \hat{\rho}_S(t) = -i[\hat{H}'_S, \hat{\rho}_S(t)] \rightarrow (3.5)$$

This equation differs from the standard Liouville–von Neumann equation for closed systems only in the use of the environment-shifted system Hamiltonian \hat{H}'_S instead of the unperturbed Hamiltonian \hat{H}_S .

Derivation of Born-Markov Equation with Born and Markov Approximation:

For this, glance over page 170- 183 (Book Number 156- 169 from 4.2.1 Structure of the Born-Markov Master Equation to 4.3 Master Equations in the Lindblad Form). Let me give a brief gist of the important assumptions. Firstly, we decompose our Hamiltonian in the following form:

$$\hat{H} = \hat{H}_s + \hat{H}_\varepsilon + \hat{H}_{int} \rightarrow (4.1)$$

We then treat \hat{H}_{int} as perturbation and $\hat{H}_0 = \hat{H}_s + \hat{H}_\varepsilon$ as unperturbed Hamiltonian. Then, just like we did for the derivation of the 1st order perturbation effects, we transform our operators and evolution in interaction picture and get an iterative solution that is of the form:

$$\frac{d}{dt} \hat{p}_s^{(I)}(t) = - \int_0^t dt' Tr_\varepsilon \left[\hat{H}_{int}(t), [\hat{H}_{int}(t'), \hat{p}^{(I)}(t')] \right] \rightarrow (4.2)$$

Equation (4.2) is the Born-Markov Equation. It is important to note that:

- $\hat{p}^{(I)}(t) = e^{i\hat{H}_0 t} \hat{p}(t) e^{-i\hat{H}_0 t}$
- $\hat{p}^{(I)}(t) = e^{i\hat{H}_0 t} e^{-iHt} \hat{p} e^{iHt} e^{-i\hat{H}_0 t} \rightarrow (4.21)$

And also:

$$\hat{H}_{int}(t) = e^{i\hat{H}_0 t} \hat{H}_{int} e^{-i\hat{H}_0 t} \rightarrow (4.22)$$

Now, the features of (4.2) that you should really emphasize upon is the following. The right-hand side of equation still depends on the total-system environment density operator $\hat{p}^{(I)}$ evaluated at all times between 0 and t and not solely in terms of $\hat{p}_s^{(I)}(t)$. To overcome these difficulties, we introduce two important assumptions: Born Approximation and Markov Approximation:

1. We would like to express our master equation entirely in terms of the reduced operator $\hat{p}_s^{(I)}(t)$ and the initial state of the environment, i.e, we would like to eliminate any terms pertaining to a time-dependent state of the environment. For this, we utilize the **Born Approximation**: The system–environment coupling is sufficiently weak and the environment is reasonably large such that changes of the density operator of the environment are negligible and the system– environment state remains in an approximate product state at all times, i.e , $\hat{p}(t) \approx \hat{p}_s(t) \otimes \hat{p}_\varepsilon$ with \hat{p}_ε constant at all times.
2. We would like to eliminate any dependences of the change of $\hat{p}_s^{(I)}$ at time t on $\hat{p}_s^{(I)}$ evaluated at times $t' < t$. The Markov approximation. “Memory effects” of the environment are negligible, in the sense that any self-correlations within the environment created by the coupling to the system decay rapidly compared to the characteristic timescale over which the state of the system varies noticeably.

Note that both approximations are motivated from the following assumptions:

- I. Weak-System environment couplings, that is, the system and the environment remain in a separable state at all times
- II. An environment that is large compared to the size of the system

Using Born-Approximation, (4.2) becomes:

$$\frac{d}{dt} \hat{\rho}_s^{(I)}(t) = - \int_0^t dt' \text{Tr}_E \left[\hat{H}_{int}(t), \left[\hat{H}_{int}(t'), \hat{\rho}_s^{(I)}(t') \otimes \hat{\rho}_E \right] \right] \rightarrow (4.3)$$

We now have that the master equation is now expressed entirely in terms of the reduced density operator $\hat{\rho}_s^{(I)}(t')$ with the state of the environment separated out and reduced to the initial state $\hat{\rho}_E$. Let us further simplify (4.3) by imposing the Markov approximation. It turns out that in many physical situation of interest, the environment can be assumed to very quickly, “forget”, any internal self-correlations that have been established in the course of the interaction with the system. In other words, in such situation the environment does not “keep track of its history”. Using Markov Approximation (4.3) becomes:

$$\frac{d}{dt} \hat{\rho}_s^{(I)}(t) = -i[\hat{H}_S, \hat{\rho}_S(t)] - \sum_{\alpha} \{ [\hat{S}_{\alpha}, B_{\alpha} \hat{\rho}_S(t)] + [\hat{\rho}_S(t) C_{\alpha}, \hat{S}_{\alpha}] \} \rightarrow (4.4)$$

Master equation in the Lindblad Form:

Master equation in the Lindblad form refer to a particular class of Markovian master equations. They arise from the requirement that the master equation ought to ensure the positivity of the reduced density matrix at all times i.e, that,

$$\langle \psi | \hat{\rho}_S(t) | \psi \rangle \geq 0 \rightarrow (4.5)$$

For any pure state $|\psi\rangle$ of the system S and for all t. It was first shown by Lindblad that the most generate master equation that satisfies condition (4.5) is of the form:

$$\frac{d}{dt} \hat{\rho}_s^{(I)}(t) = -i[\hat{H}_S, \hat{\rho}_S(t)] - \frac{1}{2} \sum_{\alpha\beta} \gamma_{\alpha\beta} \left\{ [\hat{S}_{\alpha}, \hat{\rho}_S(t) \hat{S}_{\beta}^{\dagger}] + [\hat{S}_{\alpha} \hat{\rho}_S(t), \hat{S}_{\beta}^{\dagger}] \right\} \rightarrow (4.6)$$

Canonical Models for decoherence:

Mapping Central Systems:

In many cases, the relevant dynamics of the central system can be described by one or two coordinates of interest, even if the full microscopic structure of the dynamics of system is much more complicated. These coordinates may be either continuous or discrete. An illustration of this is the ammonia molecule which we can treat as a two-level Quantum System at the expense of inner dynamics.

The physically most relevant situation involving discrete coordinates is that of a central system effectively acting as a two-level system like ammonia. This typically happens if the system has two energy minimums separated by a barrier and if the energy of the system is sufficiently low (i.e., close to the energy minimums and much less than the barrier height). Then the dynamics of the system are effectively those of a particle confined to a double-well potential. In many physical situations, besides the ground state only one or two excited states (if any) are contained in each well, and these excited states are usually not populated. Thus we obtain an effective two-state system, with the two states corresponding to localization in the “left” and “right” wells, respectively. The two levels can then in turn be mapped onto the two quantum states $|0\rangle$ (“spin up”) and $|1\rangle$ (“spin down”) of a spin-1/2 particle.

However, what if the particles, rather than just remaining in state $|0\rangle$ or $|1\rangle$ can transition between these states? That is, the particle in state $|0\rangle$ can evolve to $|1\rangle$ and the particle in state $|1\rangle$ can evolve to $|0\rangle$. In that case, taking the states $|0\rangle$ and $|1\rangle$ as the eigenstates of the Pauli z-spin operator σ_z , tunneling is mediated by:

$$\hat{H}_S^{tunnel} = -\frac{1}{2} \Delta_0 (|0\rangle\langle 1| + |1\rangle\langle 0|)$$

Where $|0\rangle\langle 1| + |1\rangle\langle 0| = \hat{\sigma}_x$ such that the tunneling term can be mediated as:

$$\hat{H}_S^{tunnel} = -\frac{1}{2} \Delta_0 (\hat{\sigma}_x) \rightarrow (5.1)$$

Ammonia molecule's wavefunction is derived in Townsend and we went through the derivation in our Quantum Mechanics II course. It assumes the form:

$$|\psi(t)\rangle = e^{-\frac{i(E_0 - A)t}{\hbar}} \left(\frac{1}{\sqrt{2}} |I\rangle + \frac{e^{-\frac{2iAt}{\hbar}}}{\sqrt{2}} |II\rangle \right) \rightarrow (5.2)$$

If we now construct the density matrix for the ammonia molecule, we have:

$$\begin{aligned}\hat{p} &= |\psi\rangle\langle\psi| = e^{-\frac{i(E_0-A)t}{\hbar}} \left(\frac{1}{\sqrt{2}} |I\rangle + \frac{e^{-\frac{2iAt}{\hbar}}}{\sqrt{2}} |II\rangle \right) e^{\frac{i(E_0-A)t}{\hbar}} \left(\frac{1}{\sqrt{2}} \langle I| + \frac{e^{\frac{2iAt}{\hbar}}}{\sqrt{2}} \langle II| \right) \\ \hat{p} &= |\psi\rangle\langle\psi| = \left(\frac{1}{\sqrt{2}} |I\rangle + \frac{e^{-\frac{2iAt}{\hbar}}}{\sqrt{2}} |II\rangle \right) \left(\frac{1}{\sqrt{2}} \langle I| + \frac{e^{\frac{2iAt}{\hbar}}}{\sqrt{2}} \langle II| \right) \\ \hat{p} &= |\psi\rangle\langle\psi| = \left(\frac{1}{2} |I\rangle\langle I| + \frac{e^{\frac{2iAt}{\hbar}}}{2} |I\rangle\langle II| + \frac{e^{-\frac{2iAt}{\hbar}}}{2} |II\rangle\langle I| + |II\rangle\langle II| \right) \rightarrow (5.3)\end{aligned}$$

Such that the overlap integral is of the form:

$$r(t) = \frac{e^{\frac{2iAt}{\hbar}}}{2} \rightarrow (5.4)$$

The density matrix assumes the form:

$$\hat{p} = \begin{pmatrix} \frac{1}{2} & \frac{1}{2} e^{\frac{2iAt}{\hbar}} \\ \frac{1}{2} e^{-\frac{2iAt}{\hbar}} & \frac{1}{2} \end{pmatrix} \rightarrow (5.5)$$

For the simple case of our density matrix, the idea of decoherence is that each time that the particle bumps with our electron, the phase $e^{i\theta}$ changes and what you measure is the *average* of these random changes. With time, the phase will average to 0 such that (5.4) will become:

$$\hat{p} = \begin{pmatrix} \frac{1}{2} & 0 \\ 0 & \frac{1}{2} \end{pmatrix} \rightarrow (5.6)$$

That is, with time, the system would lose its ability to make an interference pattern with itself.

Oscillator Environments

The representation of environments by a large number of harmonic oscillators has a long history going back to quantum electrodynamics and to spinwave and electron-gas models. Oscillator environments correspond to a quasicontinuum of delocalized bosonic field modes, with coherence and energy from the central system becoming effectively irreversibly lost into this extended bosonic environment. By “delocalized modes” we mean to convey the notion that the wave function of each harmonic oscillator (i.e., of each bosonic field mode) is spread out over a large spatial region. This delocalization of the environmental modes is a characteristic property of harmonic-oscillator environments.

Simplified Spin-Boson Model without Tunneling:

In the following, let us consider the simplified Spin-Boson Model described by the Hamiltonian:

$$\hat{H} = \hat{H}_{system} + \hat{H}_{enviornment} + \hat{H}_{interaction}$$

Since our central system is being mapped by a Spin $\frac{1}{2}$ Particle, we have that the System Hamiltonian is:

$$\hat{H}_S = \frac{1}{2} \omega_0 \sigma_z \rightarrow (6.1)$$

Where we assume there is no tunneling such a ground state $|0\rangle$ cannot transition to excited state $|1\rangle$ or excited state $|1\rangle$ transition to $|0\rangle$. Hence, we do not include $\hat{H}_S^{tunnel} = -\frac{1}{2} \Delta_0 (\hat{\sigma}_x)$. In the equation, \hat{H}_e denotes the self-Hamiltonian of the environment of Harmonic Oscillators:

$$\hat{H}_e = \sum_i \left(\frac{1}{2m_i} p_i^2 + \frac{1}{2} m\omega_i^2 q_i^2 \right) \rightarrow (6.2)$$

As established in our introductory remarks, it is σ_z coupling with the position variable that causes decoherence. In our case, we have that the interaction Hamiltonian is:

$$\hat{H}_{int} = \sigma_z \otimes \sum_i c_i \hat{q}_i \rightarrow (6.3)$$

Where equation (6.3) describes the linear coupling of the σ_z coordinate of the system to the positions coordinates \hat{q}_i of each harmonic oscillator in the environment, with coupling strengths c_i .

Finally, let us also define \hat{H}_0 as the sum of the self- Hamiltonians of the system and the environment:

$$\hat{H}_0 \equiv \hat{H}_S + \hat{H}_e$$

$$\hat{H}_0 = \frac{1}{2} \omega_0 \sigma_z + \sum_i \left(\frac{1}{2m_i} p_i^2 + \frac{1}{2} m\omega_i^2 q_i^2 \right) \rightarrow (6.4)$$

Introducing the standard bosonic annihilation and creation operators, we have:

- $\hat{q}_i = \sqrt{\frac{1}{2m_i\omega_i}} (a_i + a_i^\dagger) \rightarrow (6.41)$

- $\hat{p}_i = -i\sqrt{\frac{m_i\omega_i}{2}} (a_i - a_i^\dagger) \rightarrow (6.42)$

In terms of annihilation and creation, we can express the Hamiltonian as:

$$\hat{H} = \frac{1}{2} \omega_0 \sigma_z + \sum_i \omega_i a_i^\dagger a_i + \sigma_z \otimes \sum_i g_i a_i^\dagger + g_i^* a_i \rightarrow (6.5)$$

Note Hamiltonian is a function of σ_z and σ_z commutes with both x and p. As such,

$$[\hat{H}, \sigma_z] = 0 \rightarrow (6.6)$$

Solving the Model:

We are now going to go to interaction picture to resolve equation (6.4). In the interaction picture, we have a Time-dependent Hamiltonian $\hat{H}(t)$ that break up into two parts in the Schrodinger Picture:

$$\hat{H}(t) = \hat{H}_0 + \hat{H}_1(t) \rightarrow (6.7)$$

Where in our case,

- $\hat{H}_0 = \hat{H}_s + \hat{H}_\varepsilon = \frac{1}{2} \omega_0 \sigma_z + \sum_i \omega_i a_i^\dagger a_i \rightarrow (6.7.1)$

- $\hat{H}_1(t) = \hat{H}_{\text{int}} = \sigma_z \otimes \sum_i g_i a_i^\dagger + g_i^* a_i \rightarrow (6.7.2)$

In general, the operators O_I in interaction picture obey the following:

$$\frac{dO_I}{dt} = \frac{i}{\hbar} [\hat{H}_0, O_I] \rightarrow (6.8)$$

We then have the following important results:

- $\frac{d\sigma_z}{dt} = \frac{i}{\hbar} [\hat{H}_0, \sigma_z] = 0 \rightarrow (6.i)$
- $\frac{da_i^\dagger}{dt} = \frac{i}{\hbar} [\hat{H}_0, a_i^\dagger] = i\omega_i [a_i^\dagger a_i, a_i^\dagger] = i\omega_i a_i^\dagger \rightarrow (6.ii)$
- $\frac{da_i}{dt} = \frac{i}{\hbar} [\hat{H}_0, a_i] = i\omega_i [a_i^\dagger a_i, a_i] = -i\omega_i a_i \rightarrow (6.iii)$

From the last two, we can derive:

- $\hat{a}^\dagger(t) = e^{i\omega t} \hat{a}^\dagger \rightarrow (6.iv)$
- $\hat{a}(t) = e^{-i\omega t} \hat{a} \rightarrow (6.v)$

Using these, we aim to evaluate $\hat{H}_1(t)$ in interaction pictures. Essentially, the prescription that (i), (iv) and (v) give is to replace our annihilation and creation operators by the form (iv) and (v). Keeping that in mind, we have:

- $H_{1I} = e^{\frac{i\hat{H}_0}{\hbar}} H_1 e^{-\frac{i\hat{H}_0}{\hbar}}$
- $H_{1I} = \exp\left(\frac{i}{\hbar}\{\hat{H}_0\}\right) \sigma_z \otimes \sum_i g_i a_i^\dagger + g_i^* a_i \exp\left(\frac{i}{\hbar}\{\hat{H}_0\}\right)$
- $H_{1I} = \sigma_z \otimes \sum_i g_i \hat{a}^\dagger e^{i\omega_i t} + g_i^* a_i e^{-i\omega_i t} \rightarrow (6.9)$

We know that the time evolution can be found iteratively using Dyson Series:

$$\hat{U}_t(t) = \mathbb{1} - \frac{i}{\hbar} \int_0^t dt' \hat{H}_{1I}(t') + \left(\frac{i}{\hbar}\right)^2 \int_0^t dt' \hat{H}_{1I}(t') \int_0^{t'} dt'' \hat{H}_{1I}(t'') + \dots \rightarrow (6.10)$$

Since the commutator $[\hat{H}_{int}(t), \hat{H}_{int}(t' \neq t)]$ will in general be equal to another (time-dependent) operator, the required time ordering means that we usually cannot evaluate this series in closed form. However, a great simplification occurs in the present case. Since the commutator of the operators a_i and \hat{a}^\dagger is a c-number (instead of another operator), the commutator of $\hat{H}_{int}(t)$ and $\hat{H}_{int}(t' \neq t)$ with \hat{H}_{int} given by (9) is simply a function of c numbers. We find:

$$[\hat{H}_{int}(t), \hat{H}_{int}(t' \neq t)] = -2i \sum_i |g_i|^2 \sin \omega_i (t - t') \rightarrow (6.11)$$

The explicit evaluation is omitted by the text on the accounts of it being cumbersome. The textbook gives reference (237) for the explicit calculation. It shows:

$$\hat{U}_t(t) = e^{i\varphi(t)} \exp\left[-i \int_0^{t'} dt' \hat{H}_{1I}(t')\right] = e^{i\varphi(t)} V(t)$$