A study of a simple decoherence model

Jorge Guillén Rubio (author), J. Fernández-Rossier[1] [2] (tutor)
[1] *Departamento de Física Aplicada, Universidad de Alicante, 03690 San Vicente del Raspeig, Spain and*
[2] *International Iberian Nanotechnology Laboratory (INL), Av. Mestre José Veiga, 4715-330 Braga, Portugal*

(Dated: December 31, 2024)

In this research, we study the decoherence of a toy model describing an open quantum system formed by a qubit and a bath. For the bath, we take a particle moving in one dimension, under the influence of a potential $V_q(x)$ that depends parametrically on the state of the qubit, $q = 0, 1$. In this model, the off-diagonal terms of the qubit density matrix, that describe its quantum coherence, depend on the overlap of the wave functions of the bath evolving under V_q, namely, $\langle\psi_0(t)|\psi_1(t)\rangle$. We focus on the calculation of this quantity when $V_q(x)$ is given by a harmonic potential centered around a q dependent position.

I. INTRODUCTION

Quantum states are either coherent (pure or wave functions) or incoherent (mixed). Assigning a pure state to a quantum system implies certainty about the outcome of some measurement on that system. In the absence of outside forces or interactions, a quantum state evolves unitarily over time. Consequently, a pure quantum state remains pure. However, if the system is not perfectly isolated, for example, during a measurement, coherence is shared with the environment and appears to be lost with time. This is what we call quantum decoherence. The quantum coherence is not lost but rather mixed with many more degrees of freedom in the environment.

Decoherence can be viewed as the loss of information from a system into the environment (often modeled as a heat bath), since every system is loosely coupled with the energetic state of its surroundings.

Viewed in isolation, the system's dynamics are non-unitary (although the combined system plus environment evolves in a unitary manner). Thus the dynamics of the system alone are irreversible. As with any coupling, entanglement is generated between the system and environment.

Quantum coherence of open quantum systems is, in the vast majority of cases, fragile: as the coupling of the system increases, decoherence takes over more rapidly. There, figure of merit is the coherence time, i.e., how long does the the superposition state of two or more states of the quantum system survive when they are interacts with an environment.

As we can imagine, quantum decoherence poses a challenge to the development of the quantum technology industry. In particular, quantum computers as quantum information storage systems.

II. A MINIMAL MODEL FOR DECOHERENCE

We now try an approach that is essentially exact[1], so that we do not rely on approximations. We consider open quantum systems where the interaction with the environment is not able to change the occupations of the states of the quantum system. At $t \leq 0$ we assume the wave function of the qubit and the environment are decoupled:

$$|\Psi(t=0)\rangle = (c_0|0\rangle + |c_1|1\rangle) \otimes |\psi(0)\rangle \tag{1}$$

where c_0, c_1 are complex coefficients, $|\psi_0\rangle$ is an arbitrary state of the bath and $|0\rangle$ and $|1\rangle$ are the eigenstates of the qubit Hamiltonian, assumed to be proportional to the Pauli matrix τ_z.

At $t > 0$ the bath-qubit interaction is switched in a way that only the wave function of the environment is modified:

$$|\Psi(t>0)\rangle = \left(c_0 e^{i\epsilon_0 t}|0\rangle \otimes |\psi_0(t)\rangle\right) + \left(c_1 e^{i\epsilon_1 t}|1\rangle \otimes |\psi_1(t)\rangle\right) \tag{2}$$

Specifically, for $t = 0$ we have to have $|\psi_1(t=0)\rangle = |\psi_0(t=0)\rangle$. This is accomplished by Hamiltonians that commute with τ_z:

$$H = \frac{\Delta}{2}\tau_z \otimes 1_{N,N} + H_{\text{env},0} + V_{\text{int}}(\tau_z) \tag{3}$$

where the first term describes the qubit Hamiltonian, the second term the environment Hamiltonian and the last term a qubit-environment interaction that can only depend on τ_z, where τ_z is the Pauli matrix.

Without loss of generality, we can write:

$$V_{\text{int}}(\tau_z) = \tau_z \sum_n \lambda_n O_{\text{env,n}} \tag{4}$$

where $O_{\text{env,n}}$ are operators acting on the environment, and λ_n are a set of coupling constants. We now introduce the reduced density matrix:

$$\sigma \equiv Tr_{\text{bath}}|\Psi\rangle\langle\Psi| = \sum_{q,q'} c_q^* c_{q'} |q\rangle\langle q'|\langle\psi_{q'}|\psi_q\rangle \tag{5}$$

Also we define:

$$\mathcal{O}_{q,q'} \equiv \langle\psi_{q'}|\psi_q\rangle \tag{6}$$

So the representation of the reduced density matrix is:

$$\sigma = \begin{pmatrix} |c_0|^2 & c_0^* c_1 \mathcal{O}_{01} \\ c_1^* c_0 \mathcal{O}_{10} & |c_1|^2 \end{pmatrix} \tag{7}$$

So as we can see, the bath changes the off-diagonal terms of the reduced density matrix, i.e., it changes the relative phase between the two states, but not their probabilities. The coherence of the reduced density matrix of the qubit is given by:

$$S_{01}(t) = \mathcal{C}_{\text{isolated}}\mathcal{O}_{0,1}(t) \tag{8}$$

where

$$\mathcal{C}_{\text{isolated}} \equiv c_0^* c_1 e^{i\Delta_{01}t} \tag{9}$$

is the coherence of the isolated qubit, $\Delta_{01} = \epsilon_0 - \epsilon_1$ and

$$\mathcal{O}_{0,1}(t) \equiv \langle\psi_0(t)|\psi_1(t)\rangle \tag{10}$$

with

$$|\psi_q(t)\rangle = e^{iH(q)t}|\psi(0)\rangle \tag{11}$$

where $q = 0, 1$. In this research we work with $\mathcal{O}_{0,1}(t)$ instead of $S_{0,1}(t)$ as they are proportional.

Equation (10) describes the overlap of the environment states, at time t, evolving in the two different qubit options controls the decoherence. It is a complex number whose norm takes a maximal value of 1 at $t = 0$ and, in most instances, decays over time. In general, $\mathcal{O}_{01}(t)$ is a function of the initial state, the environment Hamiltonian, the operators O_n and the coupling constants λ_n. For a fixed finite time t, the overlap function will be decreased as the interaction with the environment, governed by λ_n, increases.

In general, we can write the environment state as a linear combination of eigenstates of the environment Hamiltonian:

$$|\psi(0)\rangle = \sum_{r_q}\psi(r_q)|r_q\rangle = \sum_{r_0}\psi(r_0)|r_0\rangle = \sum_{r_1}\psi(r_1)|r_1\rangle \tag{12}$$

where

$$H_{\text{env,q}}(\lambda)|r_q\rangle = \varepsilon_q(r)|r_q\rangle \tag{13}$$

and

$$H_{\text{env,q}} = H_{\text{env},0} + (2q-1)\lambda V_{\text{int}} \tag{14}$$

where $H_{\text{env},0}$ and V_{int} are matrices to be determined later on and λ is a dimensionless parameter that controls the strength of the qubit to the environment.

For a given *choice* of $|\psi(0)\rangle$, the coefficients $\psi(r_q)$ are determined by:

$$\langle r_q|\psi(0)\rangle = \psi(r_q) \tag{15}$$

Hence, we would write:

$$|\psi_q(t)\rangle = \sum_{r_q}\psi(r_q)e^{i\varepsilon_q(r)t}|r_q\rangle \tag{16}$$

Therefore, the decoherence induced by the coupling (entanglement) to the environment (bath), as given by eq. 10, is given by the overlap of the two states of the bath:

$$\mathcal{O}_{0,1}(t) = \sum_{r_0,r_1}\psi(r_0)^*\psi(r_1)e^{i(\varepsilon_0(r_0)-\varepsilon_1(r_1))t}\langle r_0|r_1\rangle \tag{17}$$

III. A MODEL FOR THE BATH

Our bath that is modeled by a one-dimensional harmonic potential centered around $(2q-1)\lambda x_0$, where $q = 0, 1$ describes the qubit state, λ is a dimensionless parameter that describes the strength of the qubit-bath interaction, and x_0 is the natural length scale of the harmonic oscillator, defined below. The Hamiltonian reads:

$$H_\pm = T + V_\pm = \frac{p^2}{2m} + \frac{1}{2}m\omega^2(x \pm \lambda x_0)^2 \tag{18}$$

where $\pm$ correspond to $q = +1(+)$ and $q = 0(-)$, respectively, m is the electron mass and x_0 is the classical return-point associated to the energy of the ground state:

$$\frac{1}{2}m\omega^2 x_0^2 = \frac{\hbar\omega}{2} \implies x_0 = \sqrt{\frac{\hbar}{m\omega}} \tag{19}$$

Given that the wavefunction is mostly contained in the classically allowed region, x_0 is the length scale of the spread of the wave function of the ground state of the HO.

In the next two sections we will approach to the problem both analytically and numerically.

IV. ANALYTICAL CALCULATION

In this section we sketch the analytical solution for the wave function of the environment that permits us to calculate the qubit decoherence. The Hamiltonian (18) model describes a forced harmonic oscillator. The wave function of the system can be found analytically, in terms of Glauber coherent states[2]. Here we show a small part of the lengthy development that can be found in reference[2].

A. Hamiltonian using ladder operators

We now write the Hamiltonian(s) $H_\pm$ in terms of the ladder operators. For that matter, we expand $(x\pm\lambda x_0)^2 = x^2 + \lambda^2 x_0^2 \pm 2x_0 x$ so that we have:

$$H_\pm = \hbar\omega(a^\dagger a) + \frac{1}{2}m\omega^2 x_0^2 \pm 2\left(\frac{1}{2}m\omega^2\right)\lambda x_0\sqrt{\frac{\hbar}{2m\omega}}(a+a^\dagger) \tag{20}$$

We now use eq. (19) to rewrite this as:

$$H_\pm = \hbar\omega(a^\dagger a) + \frac{1}{2}m\omega^2 x_0^2 \pm \frac{\hbar\omega}{\sqrt{2}}\lambda(a+a^\dagger) \tag{21}$$

B. Calculation of the overlap using coherent states

We now need to calculate the overlap between the states:

$$\Phi_\pm(x,t) = e^{iH_\pm t/\hbar}\Psi_0(x) \tag{22}$$

where $\Psi_0(x)$ is *the ground state of the HO with* $\lambda = 0$. For that matter, we use the next results:

$$|\Psi_\pm(t)\rangle = e^{-iH_0t/\hbar}e^{+iK_\pm(t)a^\dagger}e^{iK_\pm^*(t)a}\cdot \\ \cdot e^{-\int_0^t \frac{dK_\pm^*(s)}{ds}K_\pm(s))ds}|\Psi(0)\rangle \tag{23}$$

$$K_\pm(t) \equiv \frac{1}{\hbar}\sqrt{\frac{\hbar}{2m\omega}}\int_0^t f_\pm(s)e^{i\omega s}ds \tag{24}$$

$$f_\pm(t) = \mp\frac{\hbar\omega}{x_0}\lambda\Theta(t) \tag{25}$$

Now we use the fact that the initial state of the bath is the ground state of the HO, ie, $|\Psi(0)\rangle = |0\rangle$ and we use the definition of Glauber state, so that we can write:

$$|\Psi_\pm(t)\rangle = e^{-iH_0t/\hbar}e^{|iK_\pm(t)|^2/2}e^{-\int_0^t \frac{dK_\pm^*(s)}{ds}K_\pm(s))ds}|+iK_\pm(t)\rangle \tag{26}$$

After a lengthy algebraic manipulation, we obtain:

$$|\mathcal{O}(t)|^2 = |\langle\Psi_-(t)|\Psi_+(t)\rangle|^2 = e^{-8\lambda^2\sin^2\left(\frac{\omega t}{2}\right)} \tag{27}$$

We now take the limit or $\omega t << 1$. We thus approximate:

$$\sin\left(\frac{\omega t}{2}\right) \simeq \frac{\omega t}{2} \tag{28}$$

So, for short times, $\omega t << 1$ that we have:

$$|\mathcal{O}(t)|^2 \simeq e^{-2\lambda^2\omega^2t^2} \tag{29}$$

On the other hand, it is apparent that eq. (27) satisfies $|\mathcal{O}(t)|^2 = |\mathcal{O}(t+NT)|^2$, N is any integer number and

$$T = \frac{2\pi}{\omega} \tag{30}$$

Hence, the main takeaways from the analytical model are:

1. At short times, defined by $\omega t << 1$ the overlap that controls the qubit coherence decays as the exponential of t^2.
2. The decay is faster for larger values of λ
3. Overall, the overlap is a periodic function. Therefore, this toy model does not describe an irreversible decoherence process.

V. DISCRETIZATION OF THE SCHRÖDINGER EQUATION

We also consider a numerical solution of the Schrödinger equation of the decoherence model. This serves two purposes: first, to compare with the analytical calculation. Second, given the approximate nature of the numerical method, discussed below, to provide a second model for decoherence.

We will use the finite difference method to solve the Schrödinger equation. This is the discretization of the domain of the wave function to transform the differential equation into a linear algebra problem.

The one-dimensional time-independent Schrödinger equation is given by:

$$-\frac{\hbar^2}{2m}\frac{d^2\psi(x)}{dx^2} + V(x)\psi(x) = E\psi(x) \tag{31}$$

Our starting point is going to be the description of the wave function in a lattice of equidistant points. So we adopt the next notation for the discretized wave function and potential in a point n: $\psi(x) \to \psi(n\Delta x) \to \psi_n$ and $V(x) \to V(n\Delta x) \to V_n$, where n are integer numbers and Δx is the distance between two consecutive points. We consider that x is constraint in a simulation cell $-x_{max} \leq x \leq x_{max}$, with $\Delta x \ll x_{max}$. If we consider a lattice of N points, the wave function is described by a N-dimensional vector and the distance between two consecutive points is $\Delta x = \frac{2x_{max}}{N-1}$ and $n \in \{0, 1, ..., N-1\}$. Usually we take $N > 100$, so $\Delta x \ll x_{max}$.

The next step is translating the functional form of the Schrödinger equation into a discrete one. For this, the first step is to write the second derivative of a function in its numerical form (centered differences):

$$\frac{d^2\psi(x)}{dx^2} \approx \frac{\psi_{n+1} - 2\psi_n + \psi_{n-1}}{\Delta x^2} \tag{32}$$

Logically, the quality of this approximation depends on our choice of Δx, assuming to be small enough; this is N bigger enough.

So we see that the second derivative connects the wave function in a point n with the wave function in its two adjacent points $n \pm 1$. Now we write the Schrödinger equation in one dimension as:

$$-\frac{\hbar^2}{2m\Delta x^2}(\psi_{n+1} - 2\psi_n + \psi_{n-1}) + V_n\psi_n = E_n\psi_n \tag{33}$$

where E_n are the energies. The model of eq. (33) can be interpreted as a tight-binding model for a single quantum particle moving in a finite-size one-dimensional lattice, with first neighbor hopping and an on-site potential given by V_n.

It is convenient to realize that equation 33 describes a tridiagonal matrix eigenvalue equation, that can be solved numerically. The low energy states of eq. 33 are identical to those of the displaced harmonic oscillator. However, by virtue of the method, the high-energy states are different, unless we take an infinite simulation cell and an infinite number of points, which is of course not possible numerically. Therefore, they describe an alternative decoherence model.

VI. RESULTS

In this section we will show the results of our work. First, we need to specify the parameters chosen:

- $N_x = 1\,000$ (dimension of the $N_x \times N_x$ hamiltonian and points of the space grid)
- $x_{max} = 250\ \mathring{A}$ (half width of the simulation box)
- $N_t = 10\,000$ (points of the time grid)
- $t_{max} = \{0.1, 1\}\ ps$ (time of simulation)
- $k = 10\ meV/\mathring{A}^2$ (force constant) $\implies \omega \simeq 419\ ps^{-1}$ (frequency)
- $\lambda = \{1, 5, 10\}$ (coupling constant)

With these parameters we are able to create the matrix of the equation 33 and diagonalize it. Then we need to choose an initial state, so we select the lowest energy state of the unshifted ($\lambda = 0$) harmonic potential, i.e., a Gaussian function centered in the origin. Now are able to compute the coefficients given by the inner products of the equation 15. Then we calculate the two states as functions of time with the equation 16 to finally compute the overlap doing the inner product of the equation 17.

Having all this in mind, we present our figures for different values of the coupling constant, λ:

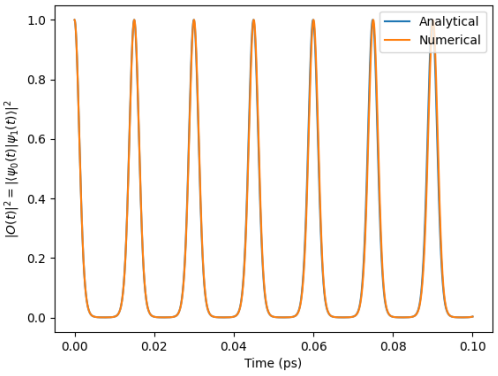

FIG. 1. Overlap modulus squared with $\lambda = 1$

In the Figure 1 we show results for the case $\lambda = 1$. We can observe that both numerical and analytical solutions match. We see a periodic overlap that ranges from e^{-8} to 1. These revivals are in agreement with equation 27, that predicts a periodic behavior for the overlap. In this scale of time, we do not observe a decay of amplitude, as after a period, both curves rise the maximum again.

We can gain some insight by inspection of the states $\psi_\pm$, computed numerically, both when the overlap is maximal ($t = 0\ ps$) and minimal, for ($t = \frac{T}{2}\ ps$):

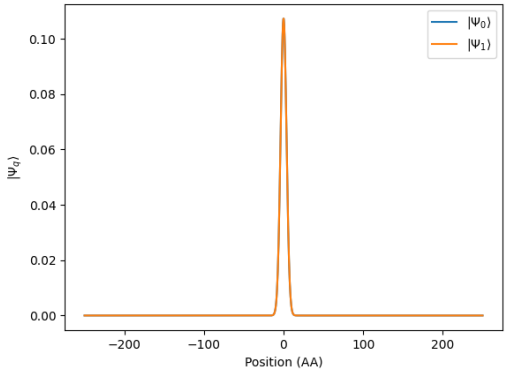

FIG. 2. States in a maximum of overlap with $\lambda = 1$

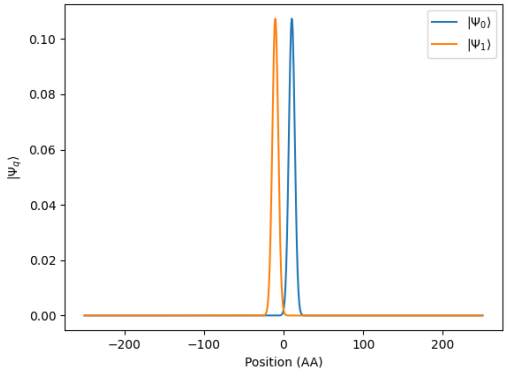

FIG. 3. States in a minimum of overlap with $\lambda = 1$

As we can see in Figure 2, when the overlap reaches its maximum, both $|\psi_0\rangle$ and $|\psi_1\rangle$ are the same. Precisely, $|\psi_0\rangle = |\psi_1\rangle = |\psi(0)\rangle$. This pattern can be understood as follows. At $t = 0$ the state of the environment is the ground state of a harmonic oscillator centered at $x = 0$. For $t \geq 0$, the wave functions $\psi_\pm$ are governed by two harmonic oscillators centered around $\mp\lambda x_0$. In a semi-classical picture, this is as we release the oscillator for a non-equilibrium position. The oscillator will excute an harmonic motion, returning to their $t = 0$ position in a synchronous manner, on account of the symmetry of the $\mp\lambda x_0$ points. The opposite happens in Figure 3, where both states are separated by $2x_0$, so the overlap is almost vanishing.

Now we show some plots where the analytical model does not match with the numerical calculation.

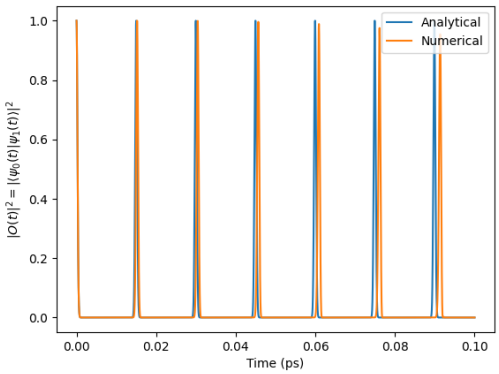

FIG. 4. Overlap modulus squared with $\lambda = 5$

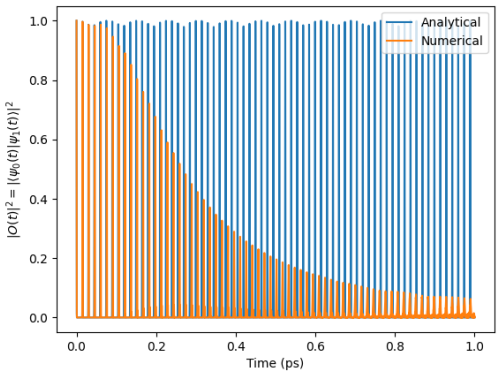

FIG. 5. Overlap modulus squared with $\lambda = 5$

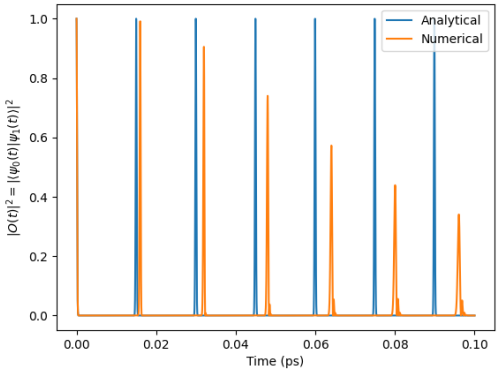

FIG. 6. Overlap modulus squared with $\lambda = 10$

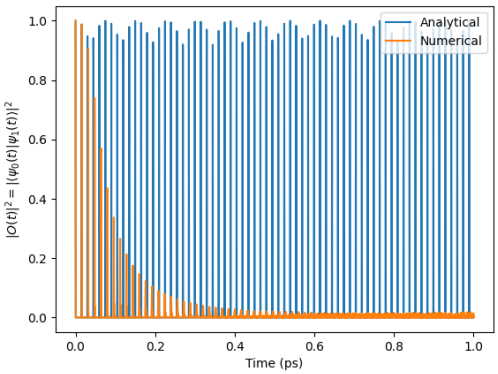

FIG. 7. Overlap modulus squared with $\lambda = 10$

As we can observe in Figure 4, 5, 6 and 7, the squared modulus of the numerical-computed overlap only reaches 1 in $t = 0$. After that moment, it oscillates as before, but the amplitude of the oscillations decays over time. It is noticeable that it decays faster as λ increases. In fact, if we wait enough time, it goes to 0 with some noise. On the other hand, the analytical function oscillates as well, but its amplitude remains almost constant in every case, and it's not exactly the same due to undersampling, as we can see in Figure 5 and 7. We can assure that because we know the function to be periodic, as shown in equation 27.

Now is time to talk about this discrepancy between our models. In fact, they are different: analytical model is based on an oscillator in an infinite box with no boundaries, and treats the states as continuous functions. On the other hand, numerical model is based on an oscillator in a box with hard walls, and treats the states as discrete functions, i.e., vectors. This also explains why numerical method differs from the analytical one for higher values of λ: because the states are closer to the walls. Additionally, both methods coincide in low energy states, but differ a lot in high energy states. As a result, the numerical model has harmonics different from $N\omega$, which allows for a more complex dynamical behavior.

VII. SUMMARY AND CONCLUSIONS

1. We have studied a simple model[1] for the decoherence of a qubit coupled to a bath. The essence of the model is that the dynamical evolution of the wave function of the bath is qubit-dependent. Hence, there are two bath states , $\psi_{\pm}$, that control the coherence of the reduced density matrix of the qubit, that is proportional to the overlap of the bath states $\langle\psi_+|\psi_-\rangle$.

2. We have computed the qubit decoherence using a bath model a 1D harmonic oscillator whose equilibrium position depends on the qubit state.

3. We have computed the decoherence both analytically and numerically. In the limit of weak and moderate coupling, the two methods give the same results. However, by virtue of approximations in the numerical method, the two methods differ for strong coupling. In this point the numerical method is actually describing a different Hamiltonian, and therefore it provides a second decoherence model.

4. For the harmonic potential, the proposed model does not describe irreversible decoherence. In contrast, in the strong-coupling limit, the numerical method describes a decay of the coherence standard in open quantum systems.

VIII. ACKNOWLEDGEMENTS

Jorge Guillén Rubio expresses his sincere gratitude to GEFES for the financial award, to Joaquín for his unwavering support and patience during countless meetings and emails, and to Yelko del Castillo for his guidance with numerical calculations. This work would not have been possible without their contributions.

[1] Ady Stern, Yakir Aharonov, and Yoseph Imry, "Phase uncertainty and loss of interference: A general picture," Physical Review A **41**, 3436 (1990).

[2] Alberto Galindo and Pedro Pascual, *Quantum mechanics I* (Springer Science & Business Media, 2012).