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Antiresonances as precursors of decoherence

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Abstract. – We show that, in the presence of a complex spectrum, antiresonances act as a precursor for dephasing enabling the crossover to a fully decoherent transport even within a unitary Hamiltonian description. This general scenario is illustrated here by focusing on a quantum dot coupled to a chaotic cavity containing a finite, but large, number of states using a Hamiltonian formulation. For weak coupling to a chaotic cavity with a sufficiently dense spectrum, the ensuing complex structure of resonances and antiresonances leads to phase randomization under coarse graining in energy. Such phase instabilities and coarse graining are the ingredients for a mechanism producing decoherence and thus irreversibility. For the present simple model one finds a conductance that coincides with the one obtained by adding a ficticious voltage probe within the Landauer-Büttiker picture. This sheds new light on how the microscopic mechanisms that produce phase fluctuations induce decoherence.

In the last decade the quantum-classical transition has been object of intense study leading to a substantial progress in its comprehension [1]. An essential ingredient is the fact that the properties of a given system, though simple, will be influenced by a hierarchy of interactions with the rest of the universe (*the environment*). However weak, such interactions lead to the degradation of the ubiquitous interference phenomena characteristic of a quantum system, *i.e.*, decoherence. Current trends in technology focus on the tailoring of such interference phenomena to achieve different goals. These range from the control of electronic currents at the nanoscale in semiconductor and molecular devices [2,3] to the flow of quantum information [4] encoded in the phase of a quantum state. The crossover between the coherent and decoherent dynamics is manifest in the behavior of the quantum phase strikingly exhibited [5] by weak localization phenomena and the Aharanov-Bohm effect. Hence, the understanding and control of the effects of the coupling to the environment on the quantum phase constitute a central problem for both, fundamental physics and practical applications.

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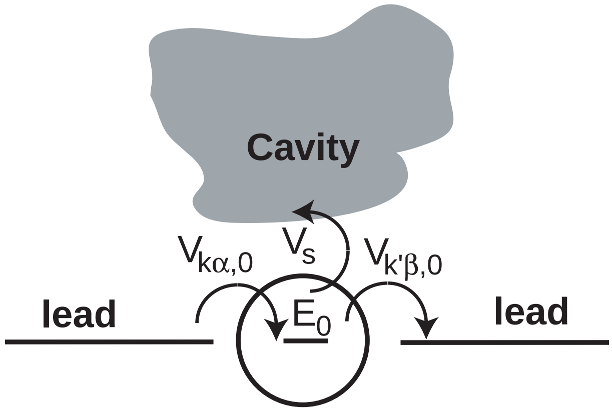

Fig. 1 – Schematic representation of the model system considered in the text: a quantum dot connected to left and right leads and to a chaotic cavity whose effect is the focus of this work.

The most obvious source of decoherence is the creation of entangled system-environment states induced by complex many-body interactions. However, recent results on the Loschmidt Echo in chaotic systems [6] have suggested that complexity is a natural road to decoherence even in a one-body problem. Indeed, once the system is complex enough there is little chance to sustain a controllable interference experiment. In this paper, we will explore the notion that, in the presence of a complex spectrum, antiresonances are a precursor for dephasing and result in decoherent transport even within a fully unitary Hamiltonian description. This is illustrated by considering a toy model for a quantum dot tunneling device coupled to a chaotic cavity containing a *large, but finite*, number of states in the energy range of interest. A possible arrangement is depicted in fig. 1. The presence of the chaotic cavity induces definite phase changes (dephasing) in the resulting wave functions. Then, our main goal will be to gain insight into how this dephasing results in the emergence of decoherence.

In what follows we will explore the effect of the coupled cavity on the phase and the transmission probability through the system. Furthermore, we will also address the consistency with Büttiker's model of decoherence [7] where the sample is coupled via a fictitious voltage probe with a reservoir whose chemical potential is set to account for current conservation. The presence of such reservoir accounts for a decoherent [8] re-injection of particles. A *Hamiltonian* formulation for this picture was proposed by D'Amato and Pastawski [9]. In that work, the connection of the dot states to an infinite system with a continuous spectrum leads to a self-energy with an imaginary part. This procedure is justified by considering decoherent electron reservoirs within the Keldysh formulation [10,11]. Here, we re-examine the latter path by exploring the consequences of the coupling with a system that contains a *finite* number of states. From this point of view, our main goal is to show how a "decoherent" behavior is an emergent phenomenon as the number of states in the chaotic cavity increases. While in our discussion we adopt a single-particle description, the conclusions will be of a general nature [12].

The total Hamiltonian is split into four terms:

$$\mathcal{H} = \mathcal{H}_{\text{dot}} + \mathcal{H}_{\text{electrodes}} + \mathcal{H}_{\text{cavity}} + \mathcal{H}_{\text{int.}}$$

The device is represented by a Hamiltonian $\mathcal{H}_{\text{dot}} + \mathcal{H}_{\text{electrodes}}$ consisting of a quantum dot that is coupled through potential barriers to the left and right electrodes. In addition, we introduce a chaotic cavity (represented by $\mathcal{H}_{\text{cavity}}$) that serves as an "environment" that perturbs the system through the coupling term contained in $\mathcal{H}_{\text{int}}$.

The dot sustains a set of states E_i whose corresponding creation and annihilation operators are $d_i^\dagger$ and d_i, respectively. This part of the Hamiltonian is written as

$$\mathcal{H}_{\text{dot}} = \sum_i E_i d_i^\dagger d_i. \tag{1}$$

The Hamiltonian for the electrodes is

$$\mathcal{H}_{\text{electrodes}} = \sum_{k,\alpha=\mathrm{L,R}} \varepsilon_{k\alpha} c_{k\alpha}^\dagger c_{k\alpha} + \sum_{k,\alpha} (V_{k\alpha,0} c_{ks}^\dagger d_0 + \text{c.c.})$$

where $c_{k\alpha}^\dagger$ represents the creation in the eigenstate k of the electrode α. The electron creation operators in an arbitrary basis for the chaotic cavity are denoted by $b_s^\dagger$,

$$\mathcal{H}_{\text{cavity}} = \sum_{s=1}^{N} \varepsilon_s b_s^\dagger b_s + \sum_{s,r}^{N} (V_{s,r} b_s^\dagger b_r + \text{c.c.}). \tag{2}$$

Without loss of generality, the coupling between the chaotic cavity and the dot is restricted to one (local) state:

$$\mathcal{H}_{\text{int}} = V_s (b_1^\dagger d_0 + \text{c.c.}).$$

In order to simplify the physics we focus our attention on a single resonance of energy E_0 which, being the closest to the Fermi energy, is relevant for transport. The matrix elements $V_{k\alpha,0}$ describe the coupling between the electrodes and the dot. The matrix elements of $\mathcal{H}_{\text{cavity}}$ are assumed to be distributed according to random matrix theory for the time-reversal invariant case (Gaussian orthogonal ensemble, GOE). The electrodes will be modeled as one-dimensional tight-binding chains with hopping V. V_L, V_R and V_s are regarded as small parameters compared with the band width of the electrodes. The electrodes can be eliminated and their effect included exactly through a self-energy (${}^L\Sigma$, ${}^R\Sigma$) [9]. After diagonalization of the matrix corresponding to $\mathcal{H}_{\text{cavity}}$, a similar procedure [13] can be applied for the "finite environment" thus obtaining a self-energy ${}^{\text{cavity}}\Sigma$. Note that in contrast to the self-energy accounting for the electrodes that contain an imaginary part, here $\text{Im}({}^{\text{cavity}}\Sigma) = 0$.

Once the self-energies are obtained, the calculation of the transmission amplitude can be carried out by computing the retarded Green's function and the group velocities at the electrodes [14]. It can be written in terms of the decay rates [9] as

$$t_{\mathrm{R,L}} = \mathrm{i}\hbar \sqrt{2^{\mathrm{R}}\Gamma}\, G_{\mathrm{R,L}}^R \sqrt{2^{\mathrm{L}}\Gamma}, \tag{3}$$

where ${}^{\mathrm{L(R)}}\Gamma = \text{Im}({}^{\mathrm{L(R)}}\Sigma)$.

In order to illustrate the basic physics of phase fluctuations, we consider the simplified case in which there are only four levels in the chaotic cavity and $\mathcal{H}_{\text{cavity}}$ corresponds to a tridiagonal matrix. In fig. 2b we show the transmission probability as a function of the energy of the incident electrons. There we can appreciate that, together with the main resonance, due to the state in the dot, there are other resonances associated with the states in the cavity. The height of these maxima is always one since the escape rates to the right and left electrodes are equal [15]. Note that the width of these resonances is decreased in comparison with the main resonance width because of the small coupling V_s. We also emphasize the presence of *antiresonances* [13,15] (*i.e.* zero-transmission points) in this log-plot. The occurrence of these antiresonances is due to a *destructive interference* between the different possible "paths" connecting the left and right electrodes. Such paths can be classified essentially as a direct path from left to right, and paths that go from the left to the right electrode passing through the chaotic cavity.

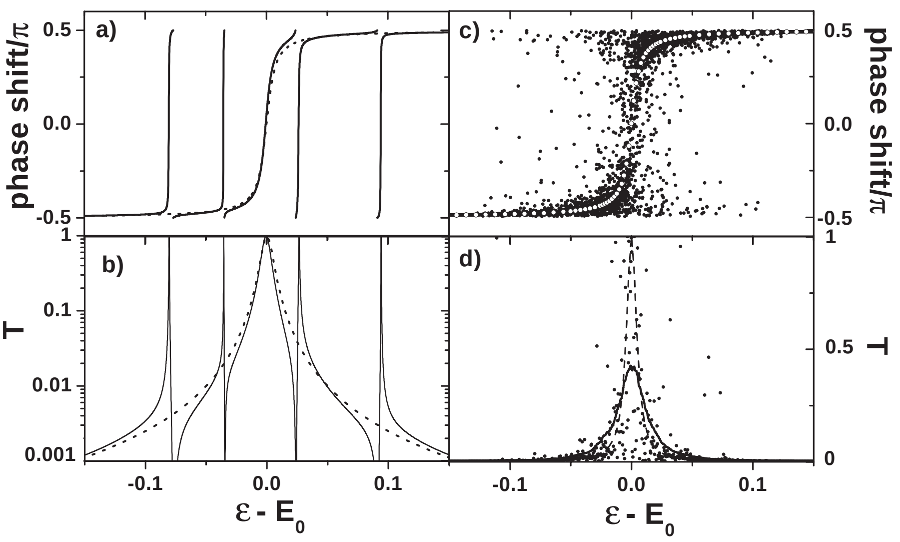

Fig. 2 – a) The phase shift as a function of the electron energy. The solid line corresponds to the total transmittance calculated using the model introduced in the text with only four states in the chaotic cavity. The parameters of the Hamiltonian in units of the hopping V in the leads are: $E_0 = 0$, $V_L = V_R = 0.05$, $V_s = 0.025$ and $\Delta_N = 0.04$. For reference, the phase shift corresponding to the situation of vanishing V_s is shown with a dashed line. In b) we show the total transmission probability as a function of the incident electron energy for the case discussed in panel a). c) Scatter plot of the phase shift as a function of the incident electron energy. The parameters of the Hamiltonian in units of the hopping V in the leads are: $E_0 = 0$, $V_L = V_R = 0.05$, $V_s = 0.02$ and $\Delta_N = 6.67 \times 10^{-5}$. In these calculations 3000 states were included in the chaotic cavity. For reference, the non-interacting phase shift is shown with circles superposed to the scatter plot. In d) we show a scatter plot of the total transmission probability. The solid line corresponds to the total transmittance calculated using the coarse-graining procedure. As in the previous figures, the dashed line corresponds to the case of zero coupling with the chaotic cavity.

Another quantity of interest is the transmission phase [16]. This quantity is accessed experimentally [17] by embedding a quantum dot in a branch of an Aharonov-Bohm interferometer. From eq. (3) the phase shift is given by

$$\theta(\varepsilon) = \frac{1}{2\mathrm{i}} \ln \left(\frac{G^R_{\mathrm{R,L}}(\varepsilon)}{G^A_{\mathrm{L,R}}(\varepsilon)} \right), \tag{4}$$

where G^A is the advanced Green's function [18]. The phase shift as a function of the electron energy is shown in fig. 2a. There, we can appreciate that at each resonance, the phase shift experiences a smooth increase of π through an energy of the order of the resonance width. On the other hand, at each antiresonance the phase shift displays an *abrupt* fall of π. This can be understood by analyzing the path followed by the transmission amplitude in the complex plane [19].

We study the case where $\mathcal{H}_{\text{cavity}}$ has a dense spectrum (characterized by a level spacing $\Delta_N \propto N^{-1}$) in the energy region close to the main resonance. The phase shift as a function of the electron energy is shown as a scatter plot in fig. 2c. The phase shift for the case of a vanishing interaction with the chaotic cavity is also shown for reference as empty circles. The same behavior observed in fig. 2a (rapid jumps of the phase) is now present but within a much smaller energy scale that is smaller than the energy resolution of the plot. For this reason the phase values appear as scattered points that give the phase at the particular energy values. If we had used a much finer resolution in energy we would see the very fine structure of the antiresonances for the dense spectrum. Due to the presence of antiresonances the phase shift is free to move between $-\pi/2$ and $\pi/2$. Hence, a small change in the energy of the incoming electron can give rise to an important change in its phase. Here the crucial point is to notice the energy is only resolved within a precision $\delta\varepsilon$ limited by the voltage bias and/or the thermal energy scale. In this range, antiresonances produce uncontrolled fluctuations of the phase. This is what is understood as dephasing, the practical impossibility to control and predict the phase of a quantum state. Seen through a transport observable this results in decoherence.

Figure 2d shows a scatter plot of the transmission probability as a function of the electron energy for 1000 energy values. For reference, the dashed curve corresponds to the situation where there is no coupling with the chaotic cavity. When coupling to the cavity is turned on, the original resonance spreads in a bundle of thinner resonances not resolved in the plot. If the spectrum of the cavity is dense enough (*i.e.*, $\Delta_N/\delta\varepsilon \ll 1$, where $\delta\varepsilon$ is a given energy resolution), the precise shape of these resonances is not only difficult to determine numerically but clearly irrelevant! We then resort to a coarse-graining procedure accounting for the natural energy resolution on the energy scale $\delta\varepsilon$, and compute the coarse-grained transmittance according to the prescription

$$\overline{T}_{\mathrm{R,L}}(\varepsilon) = \frac{1}{\delta\varepsilon}\int_{\varepsilon-\delta\varepsilon/2}^{\varepsilon+\delta\varepsilon/2} T_{\mathrm{R,L}}(\varepsilon')\mathrm{d}\varepsilon'. \tag{5}$$

In the limit of large N and small $\delta\varepsilon \gg \Delta_N$ we recover the result of ref. [9]. In fig. 2d, we show, with a solid line, the transmittance obtained using the coarse-graining procedure while the dashed line corresponds to the case $V_s = 0$. For the decoherent model [10] the transmittance, $\widetilde{T}_{\mathrm{R,L}}(\varepsilon)$, is the sum of a coherent and a decoherent term as

$$\widetilde{T}_{\mathrm{R,L}}(\varepsilon) = \frac{4\ {}^{\mathrm{R}}\Gamma\ {}^{\mathrm{L}}\Gamma}{(\varepsilon - E_0)^2 + ({}^{\mathrm{L}}\Gamma + {}^{\mathrm{R}}\Gamma + {}^{\phi}\Gamma)^2}\left\{1 + \frac{{}^{\phi}\Gamma}{{}^{\mathrm{L}}\Gamma + {}^{\mathrm{R}}\Gamma}\right\}. \tag{6}$$

The numerical result for $\overline{T}_{\mathrm{R,L}}(\varepsilon)$ coincides with $\widetilde{T}_{\mathrm{R,L}}(\varepsilon)$ hence verifying that

$$\overline{T}_{\mathrm{R,L}}(\varepsilon) \underset{\delta\varepsilon\to 0}{\longrightarrow} \widetilde{T}_{\mathrm{R,L}}(\varepsilon). \tag{7}$$

The conclusion is then that the coarse-graining prescription applied to the coherent transmittance returns the same two components as the classical application of a voltage probe to the quantum dot. Note that ${}^{\phi}\Gamma$ is determined by the Hamiltonian parameters (V_s, Δ_N, N) that can be estimated through a Fermi golden rule. We performed similar calculations for a variety of models including several energy levels and disorder in the dot consistently reproducing the results of the voltage probe models. Since these equations provide a smooth crossover from fully quantum coherent to classical incoherent transport [20], phase fluctuations due to *antiresonances emerge as a road to decoherence.*

Similar results were obtained for a variety of models of the central system coupled to single or multiple side cavities, each representing a dephasing channel, that can be addressed within the Landauer-Büttiker approach. This confirms the generality of eq. (7). Almost any model of the side cavity suffices, regardless of its chaoticity, as long as the density of states connected to the central dot is dense. The particularities of the coupling are also unimportant (in our case to a single cavity level) since this will only shift the antiresonance positions and no qualitative changes in the spectra occur. The purpose of using a random matrix as a model for the chaotic cavity is simply to avoid the appearance of particular spectral regularities that could result in specific structures (Moiré patterns) in the discrete sampling of the transmittance. In integrable systems, it might be practical to wash out possible patterns in the level spacing using a Monte Carlo procedure for the calculation of the integral. Note also that in the Landauer-Büttiker picture, the chemical potential at the ficticious probe has to be determined in order to achieve the voltmeter condition ($I_\phi = 0$). Here, the finite size of the chaotic cavity (implying $\mathrm{Im}(\Sigma_{\mathrm{cavity}}) = 0$) ensures the conservation of the steady-state current. In contrast, for a voltage probe the corresponding self-energy has a non-vanishing imaginary part. The equivalence between both models is guaranteed by the complex structure of the real part of Σ_{cavity} and the application of a coarse-graining procedure.

The above results are clearly valid for a wide range of physical situations where the essential phenomenon is wave propagation (*i.e.* electrons [5, 21], spins [22] or electromagnetic fields [23]). A hint on how the above arguments play in a full many-body problem already appears when we consider the interaction with a phonon mode. In this solvable case, one can appreciate that decoherence arises [24] because the interaction with the phonons opens several orthogonal outgoing channels for the electrons, each one differing in the number of phonons in the system [12, 25]. In this sense, our model can be thought of as a special kind of electron-phonon model where only virtual phonon emission or absorption is allowed.

In ref. [26], Stern, Aharonov and Imry argued that decoherence can be explained in terms of either a change induced by the particle in the environment that shifts it to an orthogonal state, or by a randomization of the particle's phase. In our case, we can clearly see that the coupling with the cavity is manifested in the dephasing. Besides, the idea of the bath as a generator of decoherence arises here from the impossibility to control the phase of the wave function and by restricting the energy resolution when evaluating the coarse-grained transmittance. Indeed, the maximum between the thermal uncertainty k_BT and the applied voltage provides a natural limit for the energy resolution. Experimentally, this means that if this system is placed in an arm of an Aharonov-Bohm interferometer, the crossover from the situation $\Delta_N/\delta\varepsilon \ll 1$ to $\Delta_N/\delta\varepsilon \gg 1$ should show up as an attenuation of the amplitude of the interferences.

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