Driven Tunnelling with Dissipation.

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Abstract. – We study the quantal dynamics of a harmonically driven quartic double well in the presence of dissipation. A master equation for the reduced density operator is derived in the Floquet representation. In the classical limit, this system corresponds to a Duffing oscillator with Ohmic damping. We present numerical results for the transient time evolution and for the stationary sate. The influence of the weak dissipation on interference effects in the context of driven tunnelling is discussed on the basis of these results. We find that the coherent suppression of tunnelling can be *stabilized* by reservoir-induced noise for a suitably chosen temperature.

The study of non-linear dynamics on the quantal level is centred around one basic theme: the competition of classical instabilities and fractal phase-space structures with quantum interference effects. Bistable systems under the influence of periodic driving exhibit this competition in a striking way: classically, they are characterized by the coexistence of two or more (possibly strange) attractors [1-3], while on the quantal level, they form the paradigm for coherent tunnelling. At the same time, this system class is particularly versatile—to name just a few examples: a.c.-driven SQUIDs [4, 5], laser-irradiated semiconductor double-well structures [6], laser-induced isomerization of bistable molecules [7], and paraelectric resonance [8]. Specific questions to be addressed concern, on the one hand, the influence of incoherent processes on interference effects such as the variations of tunnelling produced by driving, including its complete suppression [9-11]. On the other hand, one can ask for the modifications quantum mechanics imposes on the classical non-linear dynamics: *e.g.*, classically separate attractors will communicate through tunnelling and quantum noise, and fractal basin boundaries [12] will exhibit a lower cut-off in their fine structure. Furthermore, the phenomenon of stochastic resonance occurring in periodically driven bistable systems [13] may be brought about by quantum noise in a similar way as it is produced by classical noise.

In the present letter, we investigate a paradigmatic model, a harmonically driven quartic double well with Ohmic dissipation, corresponding, in the classical limit, to the Duffing oscillator [1-3]. There is a wealth of literature on tunnelling with dissipation [14, 15], particularly in the context of the Kramers problem [16]. In contrast to that work, however, our emphasis is on the complex spatial and temporal patterns developed by the quantal dynamics and its transition to the classical limit. Therefore, our approach is similar in spirit to that of Graham *et al.* and Haake *et al.*, respectively, on the quantal manifestations of chaos in dissipative systems [17-20]. Other systems in the same class have been studied in ref. [21-24]. In this letter, we concentrate on the discussion of the quantum-mechanical description and present a choice of first numerical results. A more detailed study is deferred to a subsequent publication [25].

The quantization of the Duffing oscillator naturally divides into two subtasks, the quantal description of an undamped driven quartic double well, and the introduction of dissipation. In the first step, we resort to Floquet theory [26-30]. It makes full use of the discrete time-translational symmetry of the Hamiltonian. Provided with the Floquet representation of the conservative system, we add dissipation by a coupling to a reservoir. Thereby, we follow closely the approach used in ref. [31].

We specify the system plus reservoir by the Hamiltonian $H(t) = H_0(t) + H_\mathrm{I} + H_\mathrm{R}$. The Hamiltonian for the driven double well reads

$$H_0(t) = \frac{p^2}{2} - \frac{x^2}{4} + \frac{x^4}{64D} + xS\cos\omega t\,. \tag{1}$$

(We use dimensionless variables throughout.) In periodically driven systems, the basic dynamical group is generated by the unitary evolution operator over one period $2\pi/\omega$ of the driving force, $U = T\exp\left[-i\int_0^{2\pi/\omega} \mathrm{d}t\, H_0(t)\right]$ (T indicates time ordering). According to the Floquet theorem, its eigenstates have the form $|\Phi_\alpha(t)\rangle = \exp[-i\varepsilon_\alpha t]|\varphi_\alpha(t)\rangle$, with $|\varphi_\alpha(t+2\pi/\omega)\rangle = |\varphi_\alpha(t)\rangle$. The *quasi-energies* ε_α have the character of phases and are therefore defined mod ω.

The interaction and reservoir Hamiltonians, respectively, are $H_\mathrm{I} = \sum_i x(g_i b_i + g_i^* b_i^\dagger)$ and $H_\mathrm{R} = \sum_i \omega_i (b_i^\dagger b_i + 1/2)$. Here b_i, $b_i^\dagger$ are the annihilation and creation operators, respectively, for a boson mode of frequency ω_i, and g_i is the corresponding coupling constant. Starting from the von-Neumann equation for the density operator of the full system, we perform the usual procedure [32-33] to trace out the reservoir degrees of freedom under the assumptions i) that driven double well and reservoir are initially uncoupled, and ii) that the reservoir is Markovian, *i.e.* correlation functions for the boson modes decay instantaneously on characteristic time scales of the double-well dynamics. We also neglect shifts of the system frequencies due to the reservoir coupling. This procedure yields a differential equation for the time evolution of the reduced density operator in the interaction picture (with respect to H_I), $\tilde{\sigma}(t)$ [31]. In order to simplify this differential equation further, we drop all oscillating contributions, *i.e.* terms corresponding to pairs of reservoir-induced transitions that virtually violate energy conservation. This approximation is analogous to the rotating-wave approximation. It is justified if the quasi-energy spectrum shows level repulsion, so that all nearest-neighbour level separations are of the order of their average. It is critical, however, and will have to be partially lifted (see below), as soon as near degeneracies, such as tunnel doublets, come into play. They introduce exceptionally slow oscillations into the equation of motion for $\tilde{\sigma}(t)$ which will not drop out upon integration. Switching to the interaction representation in the Floquet basis, we finally obtain the master equation [31]

$$\dot{\tilde{\sigma}}_{\alpha\alpha}(t) = \sum_\nu (W_{\alpha\nu}\tilde{\sigma}_{\nu\nu}(t) - W_{\nu\alpha}\tilde{\sigma}_{\alpha\alpha}(t))\,, \qquad \dot{\tilde{\sigma}}_{\alpha\beta}(t) = -\frac{1}{2}\sum_\nu (W_{\nu\alpha} + W_{\nu\beta})\tilde{\sigma}_{\alpha\beta}(t)\,, \quad \text{for } \alpha \neq \beta\,, \tag{2}$$

where $\tilde{\sigma}_{\alpha\beta}(t) = \langle\Phi_\alpha(0)|\tilde{\sigma}(t)|\Phi_\beta(0)\rangle$. The transition probabilities $W_{\alpha\beta}$ depend on the potential and the driving via the quasi-energies (which are not known analytically) as well as on the reservoir coupling and on temperature. They will be given explicitly in [25]. Equation (2) separates into two independent subsets of equations, one for the non-diagonal elements which decay exponentially, and one for the diagonal part which determines the stationary state of the system.

We briefly address two important limits of the quantal dynamics, the classical limit and the long-time limit. The classical limit (which here amounts to $D \to \infty$) can be obtained, *e.g.*, by deriving the time evolution of a (quasi-)probability distribution defined on the classical phase space, such as the Wigner distribution [34] or the Husimi function [35]. Specifying the frequency dependence of the coupling strength as $|g(\omega)|^2 = \gamma\omega/\pi(1 + \omega^2/\omega_c^2)$ we obtain, in the classical limit, the Langevin equation

$$\ddot{x} + \gamma\omega_c \int_{-\infty}^{t} dt'\, \dot{x}(t') \exp[-\omega_c(t - t')] - \frac{x}{2}(1 + 2\gamma\omega_c) + \frac{x^3}{16D} + S\cos\omega t = f(t), \qquad (3)$$

where $f(t)$ is a random force with the autocorrelation function $\langle f(t) f(t')\rangle = \gamma k_B T\omega_c \cdot \exp[-\omega_c |t - t'|]$. Equation (3) describes a Duffing oscillator with Ohmic damping and fluctuations.

The long-time limit of the density operator leads into a stationary state which is determined by the diagonal part of eq. (2) alone. In fact, stationarity in the sense of strict time independence is reached only in the Floquet representation. At finite times, the reduced density operator $\sigma(t)$ does not even possess the discrete time-translational symmetry of the Floquet states, which is retained, however, in the «stationary» state. A similar situation arises with another, more special unitary symmetry of the undamped system: the Floquet states are either even or odd under the generalized parity transformation [9] $P: x \to -x$, $p \to -p$, $t \to t + \pi/\omega$. Again, invariance under P is generally lost for the reduced density operator, but retained in its stationary state. This applies also to the corresponding classical phase-space distribution.

In fig. 1 we present the quantum dynamics generated by the master equation (2), at a parameter point ($D = 6$, $\omega = 0.9$ and $S = 0.08485$) where the driving frequency ω is close to a resonance with the transition from the ground-state doublet to the first-excited doublet in the undriven double well (*i.e.* the transition $E_2 \to E_3$), for $\gamma = 10^{-5}$ and $T = 0$. A pure, minimum-uncertainty state centred in one of the wells served as the initial state. Figure 1*a*) shows the time evolution of the autocorrelation function $P^{\sigma(0)}(t) = \mathrm{tr}[\sigma(t)\sigma(0)]/\mathrm{tr}[(\sigma(0))^2]$ at discrete times $t_n = 2\pi n/\omega$. There is a slow oscillation of $P^{\sigma(0)}(t_n)$ between 0 and 1, which corresponds, up to an augmented rate, to the familiar tunnelling, and there is a superposed fast oscillation of smaller amplitude due to the participation of quasi-energy states related to higher-lying unperturbed eigenstates. The Fourier transform of $P^{\sigma(0)}(t_n)$ yields the local spectral two-point correlation function $P_2^{\sigma(0)}(\eta)$ (see, *e.g.*, ref. [9]), a section of which is shown in fig. 1*b*): it reflects the primary effect of the incoherent processes induced by the heat bath, a broadening of the quasi-energy levels. The broadening is not uniform but lets the high-frequency components, contributed by quasi-energy pairs separated by a large quasi-energy difference, decay faster, as should be expected from the Ohmic reservoir coupling.

The spatially resolved states after 20 (graph 1), 40 (2), 8910 (3) and $5 \cdot 10^4$ (4) periods of the driving, respectively, as well as for $t \to \infty$, are presented in fig. 1*c*). While the slow oscillation ($[1, 2] \to 3$) corresponds to a flow of probability between the two potential wells, the fast oscillations are associated with transport within the wells. This transport can no longer be attributed to only a few quasi-energy states, but it still has the character of a coherent process without close similarity to the classical phase-space flow.

The stationary state, in turn (thick line in fig. 1*c*)), does bear the signature of the classical dynamics. Figure 1*d*) shows a phase-space representation of this state, in terms of the Husimi

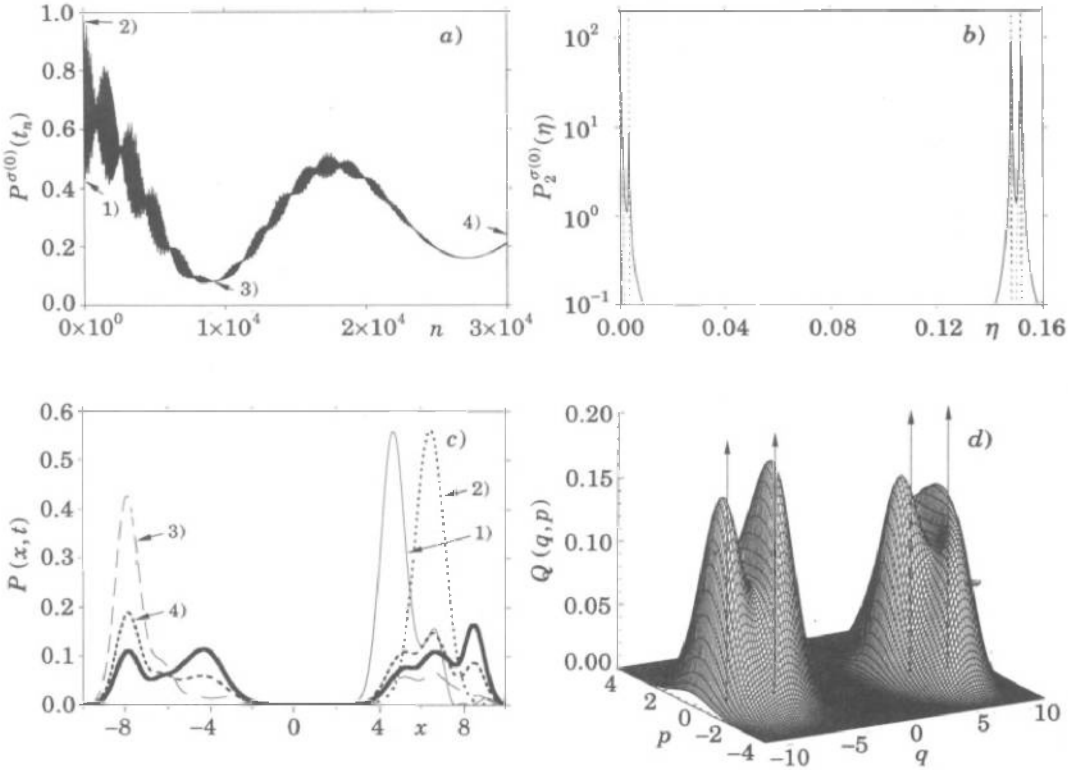

Fig. 1. – Tunnelling in the periodically driven double well with dissipation, for the parameter values $D = 6$, $\omega = 0.9$, $S = 0.08485$, $\gamma = 10^{-5}$, and $T = 0$. *a)* Time evolution of the autocorrelation function $P^{\sigma(0)}(t_n)$, with $t_n = 2\pi n/\omega$, over the first 10^4 time steps, starting from a pure, minimum-uncertainty state centred in one of the wells; *b)* a section of the Fourier transform of *a)*, corresponding to the local spectral correlation function (dashed: the same function for the undamped system); *c)* spatially resolved state at selected times t_n as marked in part *a)* (graph 1) $n = 20$, 2) $n = 40$, 3) $n = 8910$, 4) $n = 5 \cdot 10^4$) and stationary state (thick line); *d)* Husimi representation of the stationary state, compared with the corresponding classical stationary distribution (sharp peaks).

function. A comparison with the corresponding stationary state of the deterministic (*i.e.* noise-free) classical system (sharp peaks in fig. 1*d*)) demonstrates that the occurrence of two pairs of maxima (each pair rotates with the phase of the driving) coincides with the bifurcation of the classical stationary distribution into two separate point attractors (in the stroboscopic dynamics) in each well. For the present parameter values, there is a fifth classical point attractor which, however, has no discernible counterpart in the quantal stationary state.

Figure 2 is devoted to the influence of dissipation on the coherent suppression of tunnelling [9-11]. It occurs on part of the one-dimensional manifolds $\omega_{\mathrm{loc}}(S)$ in the (S, ω) parameter space where the splitting between the pair of quasi-energies corresponding to the tunnel doublet vanishes. In the vicinity of $\omega_{\mathrm{loc}}(S)$ the conservative time evolution contains very small energy scales and correspondingly large time scales. In order to still obtain an adequate description by the master equation for $\vec{\sigma}(t)$, we avoided a part of the rotating-wave approximation used in the derivation of eq. (2) by taking into account also pairs of quasi-energy transitions that virtually violate energy conservation (details will be given in ref. [25]).

Figure 2*a*) shows the time evolution of the autocorrelation $P^{\sigma(0)}(t_n)$ at a parameter point ($D = 2$, $\omega = 0.01$, $S = 3.171 \cdot 10^{-3}$) very close to, but not exactly on a manifold $\omega_{\mathrm{loc}}(S)$, for

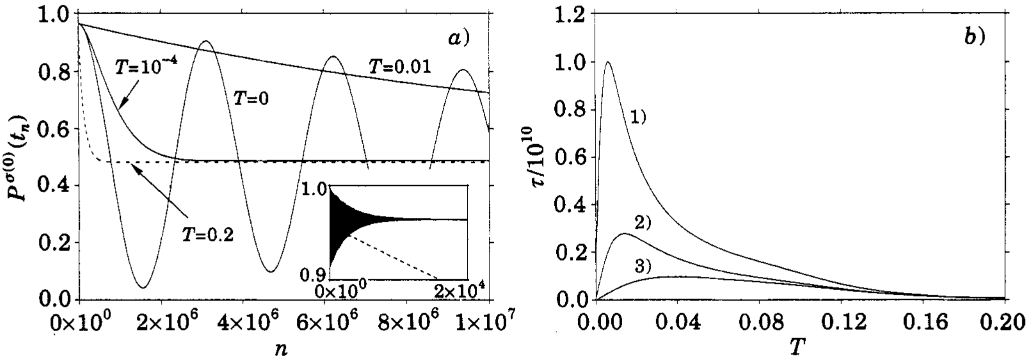

Fig. 2. – Coherent suppression of tunnelling in the presence of dissipation. *a*) Time evolution of the autocorrelation function $P^{\sigma(0)}(t_n)$, with $t_n = 2\pi n/\omega$, over the first 10^7 time steps, at a parameter point ($D = 2$, $\omega = 0.01$, and $S = 3.171 \cdot 10^{-3}$) close to a manifold where the tunnel splitting vanishes, for $\gamma = 10^{-6}$ and various values of T, starting from a pure, minimum-uncertainty state centred in one of the wells (inset: the first $2 \cdot 10^4$ time steps on an enlarged time scale); *b*) temperature dependence of the decay time τ of $P^{\sigma(0)}(t_n)$ (defined by $P^{\sigma(0)}(t_n) \sim \exp[-n/\tau]$) for three values of the detuning $\Delta\omega = \omega - \omega_{\mathrm{loc}}(S)$ from the localization manifold (graph 1) $\Delta\omega = -1.4 \cdot 10^{-7}$, as in part *a*), 2) $\Delta\omega = 5.0 \cdot 10^{-7}$ at $S = 3.1712 \cdot 10^{-3}$, 3) $\Delta\omega = 1.4 \cdot 10^{-6}$ at $S = 3.1715 \cdot 10^{-3}$). The other parameters are as in part *a*). The data shown do not extend down to $T = 0$, where $\tau(T)$ diverges, but start only with the rising part of this function.

$\gamma = 10^{-6}$ and various values of T. For low temperature, $P^{\sigma(0)}(t_n)$ exhibits a slowly decaying coherent oscillation with a very long period, due to the slight offset from $\omega_{\mathrm{loc}}(S)$. Also here, there exist superposed oscillations reflecting the admixture of other quasi-energy states. Their decay is visible only on an enlarged scale (inset in fig. 2*a*)). Asymptotically, the distribution among the wells is completely thermalized. With increasing temperature, the decay time of the slow coherent oscillation first decreases until this oscillation is suppressed from the beginning (not shown in fig. 2*b*)). After going through a minimum, however, the thermalization time increases again. At a characteristic temperature T^*, this time scale reaches a resonancelike *maximum* where the incoherent processes induced by the reservoir *stabilize* the localization of the wave packet in one of the wells and thus compensate for the detuning introduced deliberately. In fig. 2*b*), we present the temperature dependence of the decay time τ (defined by $P^{\sigma(0)}(t_n) \sim \exp[-n/\tau]$) for three values of the detuning $\Delta\omega = \omega - \omega_{\mathrm{loc}}(S)$: with increasing $\Delta\omega$, the maximum is shifted towards higher temperatures and decreases in height.

The stabilization of the coherent suppression of tunnelling by noise has already been observed in a model simpler than the present one, where the deterministic sinusoidal driving of the double well was replaced by a noisy one [36]. In fact, this phenomenon bears some resemblance both to stochastic resonance [13] and to the stabilization of instable equilibrium states by multiplicative noise [37]. It will facilitate the experimental observation of the coherent localization of driven bistable systems. A qualitative explanation, however, is not yet available.

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