12 Decoherence in Resonantly Driven Bistable Systems

Sigmund Kohler and Peter Hänggi

Institut für Physik
Universität Augsburg
86135 Augsburg
Germany

12.1 Introduction

A main obstacle for the experimental realization of a quantum computer is the unavoidable coupling of the qubits to external degrees of freedom and the decoherence caused in that way. A possible solution of this problem are error correcting codes. These, however, require redundant coding and, thus, a considerably higher algorithmic effort.

Yet another route to minimize decoherence is provided by the use of time-dependent control fields. Such external fields influence the coherent and the dissipative behavior of a quantum system and can extend coherence times significantly. One example is the stabilization of a coherent superposition in a bistable potential by coupling the system to an external dipole field [1,2]. The fact that a driving field reduces the effective level splitting and therefore decelerates the coherent dynamics as well as the dissipative time evolution is here of cruical influence. A qubit is usually represented by two distinguished levels of a more complex quantum system and, thus, a driving field may also excite the system to levels outside the doublet that forms the qubit, i.e., cause so-called leakage. While a small leakage itself may be tolerable for the coherent dynamics, its influence on the quantum coherence of the system may be even more drastic. We demonstrate in this article that in a drivien qubit resonances with higher states, which are often ignored, may in fact enhance decoherence substantially.

A related phemomenon has been found in the context of dissipative chaotic tunneling near singlet-doublet crossings where the influence of so-called chaotic levels yields an enhanced loss of coherence [3,4].

12.2 The model and its symmetries

We consider as a working model the quartic double well with a spatially homogeneous driving force, harmonic in time. It is defined by the Hamiltonian

$$H(t) = \frac{p^2}{2m} - \frac{1}{4}m\omega_0^2 x^2 + \frac{m^2\omega_0^4}{64E_\mathrm{B}}x^4 + Sx\cos(\Omega t). \tag{12.1}$$

The potential term of the static bistable Hamiltonian, H_DW, possesses two minima at $x = \pm x_0$, $x_0 = (8E_\mathrm{B}/m\omega_0^2)^{1/2}$, separated by a barrier of height E_B (cf. Fig. 12.1). The parameter

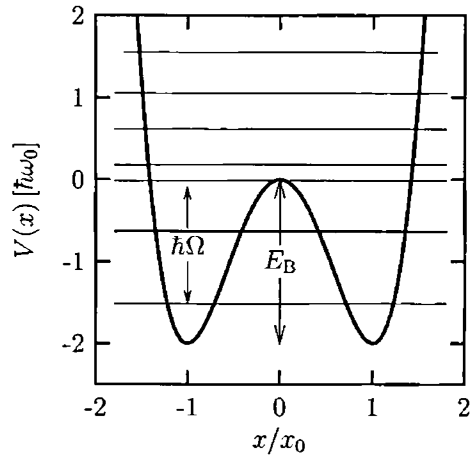

Figure 12.1: Sketch of the double well potential in Eq. (12.1) for $D = E_B/\hbar\omega_0 = 2$. The horizontal lines mark the eigenenergies in the absence of the driving; the levels below the barrier come in doublets.

ω_0 denotes the (angular) frequency of small oscillations near the bottom of each well. Thus, the energy spectrum consists of approximately $D = E_B/\hbar\omega_0$ doublets below the barrier and singlets which lie above. As a dimensionless measure for the driving strength we use $F = S(8m\omega_0^2 E_B)^{-1/2}$.

The Hamiltonian (12.1) is T-periodic, with $T = 2\pi/\Omega$. As a consequence of this discrete time-translational invariance of $H(x, p; t)$, the relevant generator of the quantum dynamics is the one-period propagator [2, 5–8]

$$U(T, 0) = \mathcal{T} \exp\left(-\frac{\mathrm{i}}{\hbar}\int_0^T \mathrm{d}t\, H_{\mathrm{DW}}(t)\right), \tag{12.2}$$

where $\mathcal{T}$ denotes time ordering. According to the Floquet theorem, the Floquet states of the system are the eigenstates of $U(T, 0)$. They can be written in the form

$$|\psi_\alpha(t)\rangle = \mathrm{e}^{-\mathrm{i}\epsilon_\alpha t/\hbar}|\phi_\alpha(t)\rangle, \tag{12.3}$$

with

$$|\phi_\alpha(t+T)\rangle = |\phi_\alpha(t)\rangle.$$

Expanded in these Floquet states, the propagator of the driven system reads

$$U(t, t') = \sum_\alpha \mathrm{e}^{-\mathrm{i}\epsilon_\alpha(t-t')/\hbar}|\phi_\alpha(t)\rangle\langle\phi_\alpha(t')|. \tag{12.4}$$

The associated eigenphases ϵ_α, referred to as quasienergies, come in classes, $\epsilon_{\alpha,k} = \epsilon_\alpha + k\hbar\Omega$, $k = 0, \pm1, \pm2, \ldots$. This is suggested by a Fourier expansion of the $|\phi_\alpha(t)\rangle$,

$$\begin{aligned} |\phi_\alpha(t)\rangle &= \sum_k |\phi_{\alpha,k}\rangle\, \mathrm{e}^{-\mathrm{i}k\Omega t}, \\ |\phi_{\alpha,k}\rangle &= \frac{1}{T}\int_0^T \mathrm{d}t\, |\phi_\alpha(t)\rangle\, \mathrm{e}^{\mathrm{i}k\Omega t}. \end{aligned} \tag{12.5}$$

The index k counts the number of quanta in the driving field. Otherwise, the members of a class α are physically equivalent. Therefore, the quasienergy spectrum can be reduced to a single "Brillouin zone", $-\hbar\Omega/2 \le \epsilon < \hbar\Omega/2$.

Since the quasienergies have the character of phases, they can be ordered only locally, not globally. A quantity that is defined on the full real axis and therefore does allow for a complete ordering, is the mean energy [2,8]

$$E_\alpha = \frac{1}{T}\int_0^T \mathrm{d}t\, \langle\psi_\alpha(t)|\, H_{\mathrm{DW}}(t)\, |\psi_\alpha(t)\rangle \tag{12.6}$$

It is related to the corresponding quasienergy by

$$E_\alpha = \epsilon_\alpha + \frac{1}{T}\int_0^T \mathrm{d}t\, \langle\phi_\alpha(t)|\, \mathrm{i}\hbar\frac{\partial}{\partial t}\, |\phi_\alpha(t)\rangle. \tag{12.7}$$

Without the driving, $E_\alpha = \epsilon_\alpha$, as it should be. By inserting the Fourier expansion (12.5), the mean energy takes the form

$$E_\alpha = \sum_k (\epsilon_\alpha + k\hbar\Omega)\, \langle\phi_{\alpha,k}|\phi_{\alpha,k}\rangle. \tag{12.8}$$

This form reveals that the kth Floquet channel yields a contribution $\epsilon_\alpha + k\hbar\Omega$ to the mean energy, weighted by the Fourier coefficient $\langle\phi_{\alpha,k}|\phi_{\alpha,k}\rangle$. For the different methods to obtain the Floquet states, we refer the reader to the reviews [2,8], and the references therein.

The invariance of the static Hamiltonian under parity $\mathsf{P} : (x,p,t) \to (-x,-p,t)$ is violated by the dipole driving force. With the above choice of the driving, however, a more general, dynamical symmetry remains. It is defined by the operation [2,8]

$$\mathsf{P}_T : (x,p,t) \to (-x,-p,t+T/2) \tag{12.9}$$

and represents a generalized parity acting in the extended phase space spanned by x, p, and phase, i.e., time $t \bmod T$. While such a discrete symmetry is of minor importance in classical physics, its influence on the quantum mechanical quasispectrum $\{\epsilon_\alpha(S,\Omega)\}$ is profound: It devides the Hilbert space in an even and an odd sector, thus allowing for a classification of the Floquet states as even or odd. Quasienergies from different symmetry classes may intersect, while quasienergies with the same symmetry typically form avoided crossings. The fact that P_T acts in the phase space extended by time $t \bmod T$, results in a particularity: If, e.g., $|\phi(t)\rangle$ is an even Floquet state, then $\exp(\mathrm{i}\Omega t)|\phi(t)\rangle$ is odd, and vice versa. Thus, two equivalent Floquet states from neighboring Brillouin zones have opposite generalized parity. This means that a classification of the corresponding solutions of the Schrödinger equation, $|\psi(t)\rangle = \exp(-\mathrm{i}\epsilon t/\hbar)|\phi(t)\rangle$, as even or odd is meaningful only with respect to a given Brillouin zone.

12.3 Coherent tunneling

With the driving switched off, $S = 0$, the classical phase space generated by H_{DW} exhibits the constituting features of a bistable Hamiltonian system: A separatrix at $E = 0$ forms the border between two sets of trajectories: One set, with $E < 0$, comes in symmetry-related pairs, each partner of which oscillates in either one of the two potential minima. The other set consists of unpaired, spatially symmetric trajectories, with $E > 0$, which encircle both wells.

Torus quantization of the integrable undriven double well implies a simple qualitative picture of its eigenstates: The unpaired tori correspond to singlets with positive energy, whereas the symmetry-related pairs below the top of the barrier correspond to degenerate pairs of eigenstates. Due to the almost harmonic shape of the potential near its minima, neighboring pairs are separated in energy approximately by $\hbar\omega_0$. Exact quantization, however, predicts that the partners of these pairs have small but finite overlap. Therefore, the true eigenstates come in doublets, each of which consists of an even and an odd state, $|\Phi_n^+\rangle$ and $|\Phi_n^-\rangle$, respectively. The energies of the nth doublet are separated by a finite tunnel splitting Δ_n. We can always choose the global relative phase such that the superpositions

$$|\Phi_n^{\mathrm{R,L}}\rangle = \frac{1}{\sqrt{2}}\left(|\Phi_n^+\rangle \pm |\Phi_n^-\rangle\right) \tag{12.10}$$

are localized in the right and the left well, respectively. As time evolves, the states $|\Phi_n^+\rangle$, $|\Phi_n^-\rangle$ acquire a relative phase $\exp(-\mathrm{i}\Delta_n t/\hbar)$ and $|\Phi_n^{\mathrm{R}}\rangle$, $|\Phi_n^{\mathrm{L}}\rangle$ are transformed into one another after a time $\pi\hbar/\Delta_n$. Thus, the particle tunnels forth and back between the wells with a frequency $\Delta_n/\hbar$. This introduces an additional, purely quantum-mechanical frequency scale, the tunneling rate $\Delta_0/\hbar$ of a particle residing in the ground-state doublet. Typically, tunneling rates are extremely small compared to the frequencies of the classical dynamics.

The driving in the Hamiltonian (12.1), even if its influence on the classical phase space is minor, can entail significant consequences for tunneling: It may enlarge the tunnel rate by orders of magnitude or even suppress tunneling altogether. For adiabatically slow driving, i.e. $\Omega \ll \Delta_0/\hbar$, tunneling is governed by the instantaneous tunnel splitting, which is always larger than its unperturbed value Δ_0 and results in an enhancement of the tunneling rate [9]. If the driving is faster, the opposite holds true: The relevant time scale is now given by the inverse of the quasienergy splitting of the ground-state doublet $\hbar/|\epsilon_1 - \epsilon_0|$. It has been found [9–11] that in this case, for finite driving amplitudes, $|\epsilon_1 - \epsilon_0| < \Delta_0$. Thus tunneling is always decelerated. When the quasienergies of the ground-state doublet (which are of different generalized parity) intersect as a function of F, the splitting vanishes and tunneling can be brought to a complete standstill by the purely coherent influence of the driving — not only stroboscopically, but also in continuous time [9–11].

So far, we have considered only driving frequencies much smaller than the frequency scale ω_0 of the relevant classical resonances. In this regime, coherent tunneling is well described within a two-state approximation [11]. Near an avoided crossing, level separations may deviate vastly, in both directions, from the typical tunnel splitting. This is reflected in time-domain phenomena ranging from the suppression of tunneling to a strong increase in its rate and to complicated quantum beats [12]. Singlet-doublet crossings, in turn, drastically change the quasienergy scales and replace the two-level by a three-level structure.

Three-level crossings

A doublet which is driven close to resonance with a singlet can be adequately described in a three-state Floquet picture. For a quantitative account of such crossings and the associated

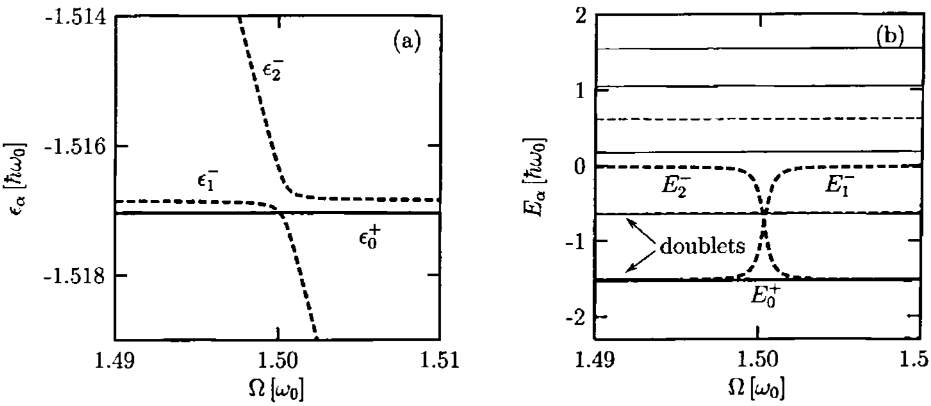

Figure 12.2: Quasienergies (a) and mean energies (b) found numerically for the driven double well potential with $D = E_B/\hbar\omega_0 = 2$ and the dimensionless driving strength $F = 10^{-3}$. Energies of states with even (odd) generalized parity are marked by full (broken) lines; bold lines (full and broken) correspond to the states (12.16) which are formed from the singlet $|\phi_t^-\rangle$ and the doublet $|\phi_d^\pm\rangle$. A driving frequency $\Omega > 1.5\,\omega_0$ corresponds to a detuning $\delta = E_t^- - E_d^- - \hbar\Omega < 0$.

coherent dynamics, and for later reference in the context of the incoherent dynamics, we shall now discuss them in terms of a simple three-state model, which has been discussed in the context of chaotic tunneling [3, 13]. In order to illustrate the above three-state model and to demonstrate its adequacy, we have numerically studied a singlet-doublet crossing that occurs for the double-well potential, Eq. (12.1), with $D = 2$, at a driving frequency $\Omega \approx 1.5\,\omega_0$ and an amplitude $F = 0.001$ (Fig. 12.2).

Far outside the crossing, we expect the following situation: There is a doublet (subscript d) of Floquet states

$$\begin{aligned} |\psi_d^+(t)\rangle &= e^{-i\epsilon_d^+ t/\hbar}|\phi_d^+(t)\rangle, \\ |\psi_d^-(t)\rangle &= e^{-i(\epsilon_d^+ + \Delta)t/\hbar}|\phi_d^-(t)\rangle, \end{aligned} \tag{12.11}$$

with even (superscript +) and odd (−) generalized parity, respectively, residing on a pair of quantizing tori in one of the well regions. We have assumed the quasienergy splitting $\Delta = \epsilon_d^- - \epsilon_d^+$ (as opposed to the unperturbed splitting) to be positive. The global relative phase is chosen such that the superpositions

$$|\phi_{R,L}(t)\rangle = \frac{1}{\sqrt{2}}\left(|\phi_d^+(t)\rangle \pm |\phi_d^-(t)\rangle\right) \tag{12.12}$$

are localized in the right and the left well, respectively, and tunnel back and forth with a frequency $\Delta/\hbar$.

As the third player, we introduce a Floquet state

$$|\psi_t^-(t)\rangle = e^{-i(\epsilon_d^+ + \Delta + \delta)t/\hbar}|\phi_t^-(t)\rangle, \tag{12.13}$$

located mainly at the top of the barrier (subscript t), so that its time-periodic part $|\phi_t^-(t)\rangle$ contains a large number of harmonics. Without loss of generality, its parity is fixed to be odd. Note that $|\phi_d^\pm(t)\rangle$ are in general not eigenstates of the static part of the Hamiltonian, but exhibit for sufficiently strong driving already a non-trivial, T-periodic time-dependence. For the quasienergy, we assume that $\epsilon_t^- = \epsilon_d^+ + \Delta + \delta = \epsilon_d^- + \delta$, where the detuning $\delta = E_t^- - E_d^- - \hbar\Omega$ serves as a measure of the distance from the crossing. The mean energy of $|\psi_t^-(t)\rangle$ lies approximately by $\hbar\Omega$ above the doublet such that $|E_d^- - E_d^+| \ll E_t^- - E_d^\pm$.

In order to model an avoided crossing between $|\phi_d^-\rangle$ and $|\phi_t^-\rangle$, we suppose that there is a non-vanishing fixed matrix element

$$b = \frac{1}{T}\int_0^T \mathrm{d}t\, \langle\phi_d^-|H_{\mathrm{DW}}|\phi_t^-\rangle > 0. \tag{12.14}$$

For the singlet-doublet crossings under study, we typically find that $\Delta \lesssim b \ll \hbar\Omega$. Neglecting the coupling with all other states, we model the system by the three-state (subscript 3s) Floquet Hamiltonian [3,4]

$$\mathcal{H}_{3s} = \epsilon_d^+ + \begin{pmatrix} 0 & 0 & 0 \\ 0 & \Delta & b \\ 0 & b & \Delta+\delta \end{pmatrix} \tag{12.15}$$

in the three-dimensional Hilbert space spanned by $\{|\phi_r^+(t)\rangle, |\phi_d^-(t)\rangle, |\phi_t^-(t)\rangle\}$. Its Floquet states are

$$\begin{aligned} |\phi_0^+(t)\rangle &= |\phi_d^+(t)\rangle, \\ |\phi_1^-(t)\rangle &= \left(|\phi_d^-(t)\rangle\cos\beta - |\phi_t^-(t)\rangle\sin\beta\right), \\ |\phi_2^-(t)\rangle &= \left(|\phi_d^-(t)\rangle\sin\beta + |\phi_t^-(t)\rangle\cos\beta\right). \end{aligned} \tag{12.16}$$

with quasienergies

$$\epsilon_0^+ = \epsilon_d^+, \quad \epsilon_{1,2}^- = \epsilon_d^+ + \Delta + \frac{1}{2}\delta \mp \frac{1}{2}\sqrt{\delta^2 + 4b^2}, \tag{12.17}$$

and mean energies, neglecting contributions of the matrix element b,

$$\begin{aligned} E_0^+ &= E_d^+, \\ E_1^- &= E_d^-\cos^2\beta + E_t^-\sin^2\beta, \\ E_2^- &= E_d^-\sin^2\beta + E_t^-\cos^2\beta. \end{aligned} \tag{12.18}$$

The angle β describes the mixing between the Floquet states $|\phi_d^-\rangle$ and $|\phi_t^-\rangle$ and is an alternative measure of the distance to the avoided crossing. By diagonalizing the matrix (12.15), we obtain

$$2\beta = \arctan\left(\frac{2b}{\delta}\right), \quad 0 < \beta < \frac{\pi}{2}. \tag{12.19}$$

For $\beta \longrightarrow \pi/2$, corresponding to $-\delta \gg b$, we retain the situation far right of the crossing, as outlined above, with $|\phi_1^-\rangle \approx -|\phi_t^-\rangle$, $|\phi_2^-\rangle \approx |\phi_d^-\rangle$. To the far left of the crossing, i.e. for

$\beta \to 0$ or $\delta \gg b$, the exact eigenstates $|\phi_1^-\rangle$ and $|\phi_2^-\rangle$ have interchanged their shape [3, 12]. Here, we have $|\phi_1^-\rangle \approx |\phi_d^-\rangle$ and $|\phi_2^-\rangle \approx |\phi_t^-\rangle$. The mean energy is essentially determined by this shape of the state, so that there is also an exchange of E_1^- and E_2^- in an exact crossing, cf. Eq. (12.18), while E_0^+ remains unaffected (Fig. 12.2b).

To study the dynamics of the tunneling process, we focus on the state

$$|\psi(t)\rangle = \frac{1}{\sqrt{2}}\left(\mathrm{e}^{-\mathrm{i}\epsilon_0^+ t/\hbar}|\phi_0^+(t)\rangle + \mathrm{e}^{-\mathrm{i}\epsilon_1^- t/\hbar}|\phi_1^-(t)\rangle\cos\beta + \mathrm{e}^{-\mathrm{i}\epsilon_2^- t/\hbar}|\phi_2^-(t)\rangle\sin\beta\right). \tag{12.20}$$

It is constructed such that at $t = 0$, it corresponds to the decomposition of $|\phi_\mathrm{R}\rangle$ in the basis (12.16) at finite distance from the crossing. Therefore, it is initially localized in the right well and follows the time evolution under the Hamiltonian (12.15). From Eqs. (12.12), (12.16), we find the probabilities for its evolving into $|\phi_\mathrm{R}\rangle$, $|\phi_\mathrm{L}\rangle$, or $|\phi_\mathrm{t}\rangle$, respectively, to be

$$\begin{aligned}
P_{\mathrm{R,L}}(t) &= |\langle\phi_{\mathrm{R,L}}(t)|\psi(t)\rangle|^2 \\
&= \frac{1}{2}\left(1 \pm \left[\cos\frac{(\epsilon_1^- - \epsilon_0^+)t}{\hbar}\cos^2\beta + \cos\frac{(\epsilon_2^- - \epsilon_0^+)t}{\hbar}\sin^2\beta\right]\right. \\
&\quad \left. + \left[\cos\frac{(\epsilon_1^- - \epsilon_2^-)t}{\hbar} - 1\right]\cos^2\beta\sin^2\beta\right), \qquad (12.21) \\
P_\mathrm{t}(t) &= |\langle\phi_\mathrm{t}(t)|\psi(t)\rangle|^2 = \left[1 - \cos\frac{(\epsilon_1^- - \epsilon_2^-)t}{\hbar}\right]\cos^2\beta\sin^2\beta.
\end{aligned}$$

At sufficient distance from the crossing, there is only little mixing between the doublet and the resonant states, i.e., $\sin\beta \ll 1$ or $\cos\beta \ll 1$. The tunneling process then follows the familiar two-state dynamics involving only $|\phi_d^+\rangle$ and $|\phi_d^-\rangle$, with tunnel frequency $\Delta/\hbar$. Close to the avoided crossing, $\cos\beta$ and $\sin\beta$ are of the same order of magnitude, and $|\phi_1^-\rangle$, $|\phi_2^-\rangle$ become very similar to one another. Each of them has now support at the barrier top and in the well region, they are of a hybrid nature. Here, the tunneling involves all the three states and must be described at least by a three-level system. The exchange of probability between the two well regions proceeds via a "stop-over" at hte top of the barrier.

12.4 Dissipative tunneling

The small energy scales associated with tunneling make it extremely sensitive to any loss of coherence. As a consequence, the symmetry underlying the formation of tunnel doublets is generally broken, and an additional energy scale is introduced, the effective finite width attained by each discrete level. As a consequence, the familiar way tunneling fades away in the presence of dissipation on a time scale t_coh. In general, this time scale gets shorter for higher temperatures, reflecting the growth of the transition rates. However, there exist counterintuitive effects: in the vicinity of an exact crossing of the ground-state doublet, coherence can be stabilized with higher temperatures [1] until levels outside the doublet start to play a role.

As a measure for the coherence of a quantum system we employ in this work the Renyi entropy [14]

$$S_\alpha = \frac{\ln \operatorname{tr} \rho^\alpha}{1-\alpha}. \tag{12.22}$$

In our numerical studies we will use S_2 which is related to the purity $\operatorname{tr}(\rho^2)$. It possesses a convenient physical interpretation: Suppose that ρ describes an incoherent mixture of n states with equal probability, then $\operatorname{tr}(\rho^2)$ reads $1/n$ and one accordingly finds $S_2 = \ln n$.

Floquet-Markov master equation

To achieve a microscopic model of dissipation, we couple the driven bistable system (12.1) bilinearly to a bath of non-interacting harmonic oscillators [8, 15, 16]. The total Hamiltonian of system and bath is then given by

$$H(t) = H_{\mathrm{DW}}(t) + \sum_{\nu=1}^{\infty} \left(\frac{p_\nu^2}{2m_\nu} + \frac{m_\nu}{2}\omega_\nu^2 \left(x_\nu - \frac{g_\nu}{m_\nu \omega_\nu^2} x \right)^2 \right). \tag{12.23}$$

Due to the bilinearity of the system-bath coupling, one can eliminate the bath variables to get an exact, closed integro-differential equation for the reduced density matrix $\rho(t) = \operatorname{tr}_{\mathrm{B}} \rho_{\mathrm{total}}(t)$. It describes the dynamics of the central system, subject to dissipation.

In the case of weak coupling, such that the dynamics is predominatly coherent, the reduced density operator obeys in good approximation a Markovian master equation. The Floquet states $|\phi_\alpha(t)\rangle$ form then a well-adapted basis set for a decomposition that allows for an efficient numerical treatment. If the spetral density of the bath influence is ohmic [8, 16], the resulting master equation reads [17, 18]

$$\dot{\rho}_{\alpha\beta}(t) = -\frac{\mathrm{i}}{\hbar}(\epsilon_\alpha - \epsilon_\beta)\rho_{\alpha\beta}(t) + \sum_{\alpha'\beta'} \mathcal{L}_{\alpha\beta,\alpha'\beta'}\rho_{\alpha'\beta'}. \tag{12.24}$$

The time-independent dissipative kernel

$$\begin{aligned} \mathcal{L}_{\alpha\beta,\alpha'\beta'} &= \sum_k (N_{\alpha\alpha',k} + N_{\beta\beta',k}) X_{\alpha\alpha',k} X_{\beta'\beta,-k} \\ &\quad -\delta_{\beta\beta'} \sum_{\beta'',k} N_{\beta''\alpha',k} X_{\alpha\beta'',-k} X_{\beta''\alpha',k} \\ &\quad -\delta_{\alpha\alpha'} \sum_{\alpha''k} N_{\alpha''\beta',k} X_{\beta'\alpha'',-k} X_{\alpha''\beta,k} \end{aligned} \tag{12.25}$$

is given by the Fourier coefficients of the position matrix elements,

$$X_{\alpha\beta,k} = \frac{1}{T}\int_0^T \mathrm{d}t\, \mathrm{e}^{-\mathrm{i}k\Omega t} \langle \phi_\alpha(t)|x|\phi_\beta(t)\rangle\rangle = X^*_{\beta\alpha,-k} \tag{12.26}$$

and the coefficients

$$N_{\alpha\beta,k} = N(\epsilon_\alpha - \epsilon_\beta + k\hbar\Omega), \quad N(\epsilon) = \frac{m\gamma\epsilon}{\hbar^2} \frac{1}{\mathrm{e}^{\epsilon/k_{\mathrm{B}}T} - 1} \tag{12.27}$$

which consist basically of the spectral density times the thermal occupation of the bath.

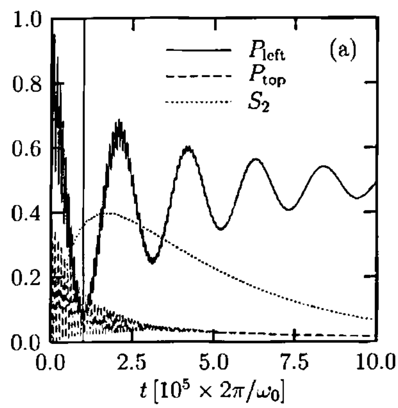

Figure 12.3: Time evolution of the state $|\phi_{\rm L}\rangle$ at the center of the singlet-doublet crossing found for $D = 2$, $F = 10^{-3}$, and $\Omega = 1.5\,\omega_0$. The full line depicts the return probability and the broken line the occupation probability of the state at the top of the barrier. The dotted line marks the Renyi entropy S_2. Panel (b) is a blow-up of the marked region on the left of panel (a).

Dissipative time evolution

We have studied dissipative tunneling at the particular singlet-doublet crossing introduced in Sec. 12.3 (see Fig. 12.2). The time evolution has been computed numerically by integrating the master equation (12.24). As initial condition, we have chosen the density operator $\rho(0) = |\phi_{\rm L}\rangle\langle\phi_{\rm L}|$, i.e. a pure state located in the left well.

In the vicinity of a singlet-doublet crossing, the tunnel splitting increases and during the tunneling, the singlet $|\phi_{\rm t}\rangle$ at the top of the barrier becomes populated periodically with frequency $|\epsilon_2^- - \epsilon_1^-|/\hbar$, cf. Eq. (12.21) and Fig. 12.3b. The large mean energy of this singlet results in an enhanced entropy production at times when it is well populated (dashed and dotted line in Fig. 12.3b). For the relaxation towards the asymptotic state, also the slower transitions within doublets are relevant. Therefore, the corresponding time scale can be much larger than $t_{\rm coh}$ (dotted line in Fig. 12.3a).

To obtain quantitative estimates for the dissipative time scales, we approximate $t_{\rm coh}$ by the growth of the Renyi entropy, averaged over a time $t_{\rm p}$,

$$\frac{1}{t_{\rm coh}} = \frac{1}{t_{\rm p}} \int_0^{t_p} {\rm d}t'\dot{S}_2(t') = \frac{1}{t_{\rm p}}\Big(S_2(t_p) - S_2(0)\Big)\,. \tag{12.28}$$

Because of the stepwise growth of the Renyi entropy (Fig. 12.3b), we have chosen the propagation time $t_{\rm p}$ as an n-fold multiple of the duration $2\pi\hbar/|\epsilon_2^- - \epsilon_1^-|$ of a tunnel cycle. For this procedure to be meaningful, n should be so large that the Renyi entropy increases substantially during the time $t_{\rm p}$ (in our numerical studies from zero to a value of approximately 0.2). We find that at the center of the avoided crossing, the decay of coherence, respectively the entropy growth, becomes much faster and is essentially independent of temperature (Fig. 12.4a). At a temperature $k_{\rm B}T = 10^{-4}\hbar\omega_0$ it is enhanced by three orders of magnitude. This indicates that transitions from states with mean energy far above the ground state play a crucial role.

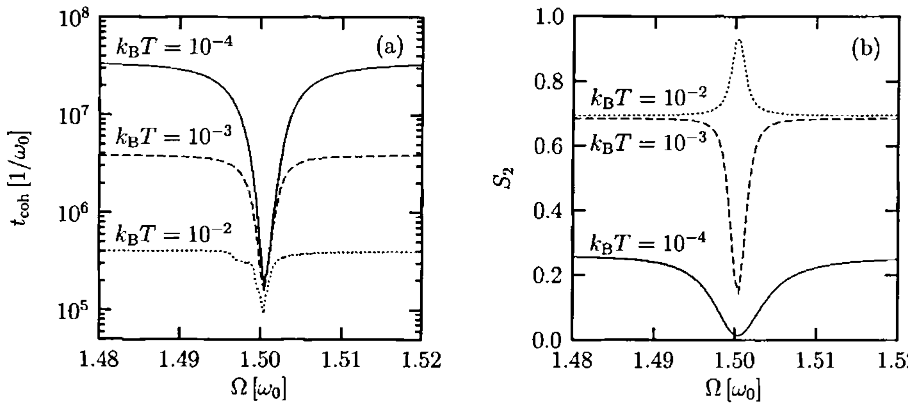

Figure 12.4: Decoherence time (a) and Renyi entropy S_2 of the asymptotic state (b) in the vicinity of the singlet-doublet crossing for $D = 2$, $F = 10^{-3}$, and $\Omega = 1.5\,\omega_0$. The temperature is given in units of $\hbar\omega_0$.

As the dynamics described by the master equation (12.24) is dissipative, it converges in the long-time limit to an asymptotic state $\rho_\infty(t)$. In general, this attractor remains time dependent but shares the symmetries of the central system, i.e. here, periodicity and generalized parity. However, the coefficients (12.25) of the master equation for the matrix elements $\rho_{\alpha\beta}$ are time independent and so the asymptotic solution also is. The explicit time dependence of the attractor has been effectively eliminated by the use of a Floquet basis.

To gain some qualitative insight into the asymptotic solution, we focus on the diagonal elements

$$\mathcal{L}_{\alpha\alpha,\alpha'\alpha'} = 2\sum_n N_{\alpha\alpha',n}|X_{\alpha\alpha',n}|^2, \quad \alpha \neq \alpha', \tag{12.29}$$

of the dissipative kernel. They give the rates of direct transitions from $|\phi_{\alpha'}\rangle$ to $|\phi_\alpha\rangle$. Within a golden rule description, these were the only non-vanishing contributions to the master equation to affect the diagonal elements $\rho_{\alpha\alpha}$ of the density matrix.

In the case of zero driving amplitude, the Floquet states $|\phi_\alpha\rangle$ reduce to the eigenstates of the undriven Hamiltonian H_{DW}. The only non-vanishing Fourier component is then $|\phi_{\alpha,0}\rangle$, and the quasienergies ϵ_α reduce to the corresponding eigenenergies E_α. Thus $\mathcal{L}_{\alpha\alpha,\alpha'\alpha'}$ only consists of a single term proportional to $N(E_\alpha - E_{\alpha'})$. It describes two kinds of thermal transitions: decay to states with lower energy and, if the energy difference is less than k_BT, thermal activation to states with higher energy. The ratio of the direct transitions forth and back then reads

$$\frac{\mathcal{L}_{\alpha\alpha,\alpha'\alpha'}}{\mathcal{L}_{\alpha'\alpha',\alpha\alpha}} = \exp\left(-\frac{E_\alpha - E_{\alpha'}}{k_BT}\right). \tag{12.30}$$

We have detailed balance and therefore the steady-state solution is

$$\rho_{\alpha\alpha'}(\infty) \sim \mathrm{e}^{-E_\alpha/k_BT}\,\delta_{\alpha\alpha'}. \tag{12.31}$$

In particular, the occupation probability decays monotonically with the energy of the eigenstates. In the limit $k_B T \to 0$, the system tends to occupy mainly the ground state.

For a strong driving, each Floquet state $|\phi_\alpha\rangle$ contains a large number of Fourier components and $\mathcal{L}_{\alpha\alpha,\alpha'\alpha'}$ is given by a sum over contributions with quasienergies $\epsilon_\alpha - \epsilon_{\alpha'} + k\hbar\Omega$. Thus, a decay to states with "higher" quasienergy (recall that quasienergies do not allow for a global ordering) becomes possible due to terms with $k < 0$. Physically, it amounts to an incoherent transition under absorption of driving-field quanta. Correspondingly, the system tends to occupy Floquet states comprising many Fourier components with low index k. According to Eq. (12.8), these states have a low mean energy.

The effects under study are found for a driving with a frequency of the order ω_0. Thus, for a quasienergy doublet, not close to a crossing, we have $|\epsilon_\alpha - \epsilon_{\alpha'}| \ll \hbar\Omega$, and $\mathcal{L}_{\alpha'\alpha',\alpha\alpha}$ is dominated by contributions with $n < 0$, where the splitting has no significant influence. However, except for the tunnel splitting, the two partners in the quasienergy doublet are almost identical. Therefore, with respect to dissipation, both should behave similarly. In particular, one expects an equal population of the doublets even in the limit of zero temperature in contrast to the time-independent case.

In the vicinity of a singlet-doublet crossing the situation is more subtle. Here, the odd partner, say, of the doublet mixes with the singlet, cf. Eq. (12.16), and thus acquires components with higher energy. Due to the high mean energy E_t^- of the singlet, close to the top of the barrier, the decay back to the ground state can also proceed indirectly via other states with mean energy below E_t^-. Thus, $|\phi_1^-\rangle$ and $|\phi_2^-\rangle$ are depleted and mainly $|\phi_0^+\rangle$ will be populated. However, if the temperature is significantly above the splitting $2b$ at the avoided crossing, thermal activation from $|\phi_0^+\rangle$ to $|\phi_{1,2}^-\rangle$, accompanied by depletion via the states below E_t^-, becomes possible. Asymptotically, all these states become populated in a cyclic flow.

In order to characterize the coherence of the asymptotic state, we use again the Renyi entropy (12.22). According to the above scenario, we expect S_2 to assume the value $\ln 2$, in a regime with strong driving but preserved doublet structure, reflecting the incoherent population of the ground-state doublet. In the vicinity of the singlet-doublet crossing where the doublet structure is dissolved, its value should be of the order unity for temperatures $k_B T \ll 2b$ and much less than unity for $k_B T \gg 2b$ (Fig. 12.4b). This means that the crossing of the singlet with the doublet leads asymptotically to an improvement of coherence if the temperature is below the splitting of the avoided crossing. For temperatures above the splitting, the coherence becomes derogated. This phenomenon compares to chaos-induced coherence or incoherence, respectively, found in Ref. [3] for dissipative chaos-assisted tunneling.

12.5 Conclusions

For the generic situation of the dissipative quantum dynamics of a particle in a driven double-well potential, resonances play a significant role for the loss of coherence. The influence of states with higher energy alters the splittings of the doublets and thus the tunneling rates. We have studied decoherence in the vicinity of crossings of singlets with tunnel doublets under the influence of an environment. As a simple intuitive model to compare against, we have constructed a three-state system which in the case of vanishing dissipation, provides a faithful description of an isolated singlet-doublet crossing. The center of the crossing is characterized by a strong mixing of the singlet with one state of the tunnel doublet. The high mean energy of the singlet introduces additional decay channels to states outside the three-state system. Thus, decoherence becomes far more effective and, accordingly, coherent oscillations fade away on a much shorter time scale.

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