

Chapter 4

Dissipation in Quantum Mechanical Systems: Where Is the System and Where Is the Reservoir?

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4.1 Introduction

Brownian motion, that is the fate of a heavy particle immersed in a fluid of lighter particles, is *the* prototype of a dissipative system coupled to a thermal bath with infinitely many degrees of freedom. The work by Einstein in (1905) developed a mathematical language to describe the random motion of the particle and uncovered the fundamental relation between friction, diffusion, and the temperature T of the bath. Half a century later, this seed had grown into the theory of irreversible thermodynamics (Landau and Lifshitz 1958), which governs the relaxation and fluctuations of classical systems near equilibrium. By that time, a new challenge had emerged, the quantum mechanical description of dissipative systems.

In contrast to classical Brownian motion, where right from the beginning the work by Einstein and Smoluchowski (Smoluchowski 1906) had provided a way to consider both weak and strong friction, the quantum mechanical theory could for a long time only handle the limit of weak dissipation. In this case the interaction between the “particle” and the “bath” can be treated perturbatively and one can derive a master equation for the reduced density matrix of the “particle” (Blum 1981). This approach has been very successful in quite a number of fields emerging in the 1950s and 1960s, such as nuclear magnetic resonance (Wangsness and Bloch 1953; Redfield 1957) and quantum optics (Gardiner and Zoller 2004). It turns out that, in this regime, conventional concepts developed in classical thermodynamics still apply, since the “particle” can be considered as a basically independent entity while the role of the reservoir is to induce decoherence and relaxation towards a thermal Boltzmann distribution solely determined (apart from temperature) by properties of the “particle”.

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Roughly speaking, a dissipative quantum system can be characterized by three typical energy scales: an excitation energy $\hbar\omega_0$, where ω_0 is a characteristic frequency of the system, a coupling energy $\hbar\gamma$ to the bath, where γ is a typical damping rate, and the thermal energy $k_B T$. The weak coupling master equation is limited to the region $\hbar\gamma \ll \hbar\omega_0, k_B T$. This is the case whenever the typical linewidth caused by environmental interactions is small compared to the line separation and the thermal “Matsubara” frequency $2\pi k_B T/\hbar$.

It is thus to be expected that, for stronger damping and/or lower temperatures, quantum mechanical non-locality may have a profound impact on the system- (“particle”) bath correlation. With the further progress in describing the system-bath interaction non-perturbatively in terms of path integrals (Weiss 2008), it has turned out that this is indeed the case. In fact, quantum Brownian motion in this regime gives rise to collective processes that cannot be understood from those of the independent parts (emergence). Accordingly, the concept of “reduction” on which the formulation of open quantum systems is based, wherein one concentrates on a relevant system and keeps from the actual reservoir only its effective impact on this system, appears in a new light. In particular, while the procedure has been extremely successful, it forces us to abandon conventional perceptions about the role of what we consider as the “system” and what we consider as the “surroundings”. The goal of the present contribution is to illustrate and discuss this situation.

To set the stage, I will start by briefly recalling the formulation of noisy classical dynamics and then proceed with a discussion about the general formulation of open quantum systems. The three specific examples to follow illustrate various facets of the intricate correlations between a system and its reservoir. As such they may also reveal new aspects of the concatenation between quantum system and observer.

4.2 Dissipation and Noise in Classical Systems

Energy dissipation in classical systems is a well-known phenomenon. A prominent example is the dynamics of a damped pendulum: starting initially from an elongated position, one observes an irreversible energy flow out of the system which finally brings it back to its equilibrium state. A more subtle situation is the diffusive motion of a small particle immersed in a liquid, also known as Brownian motion. As first pointed out by Einstein (1905), the stochastic movement of the small particle directly reflects scattering processes with the molecules of the thermal environment. In a stationary situation, the energy gained/lost in each scattering event is balanced by an energy flow into/out of this thermal reservoir. A brute force description of Brownian motion would start from Newton’s equation of motion for the whole compound system, small particle and molecules in the liquid. From a purely practical point of view, this is completely out of reach, not only due to the enormous number of degrees of freedom but also owing to the fact that microscopic details of the molecule–molecule and molecule–particle interaction are not usually known in detail. However, even if this information were available and even if we

were able to simulate the complex dynamics numerically, what would we learn if we were only interested in the motion of the immersed particle? The relevant information would have to be extracted from a huge pile of data and the relevant mechanism governing the interaction between particle and liquid would basically remain hidden.

Hence, the standard approach is based on Newton's equation of motion for the relevant particle augmented by forces describing both dissipative energy flow and stochastic scattering. For a one-dimensional particle of mass m and position q moving in a potential field $V(q)$, this leads in the simplest case to a so-called Langevin equation (Risken 1984):

$$m\ddot{q}(t) + V'(q) + m\gamma\dot{q}(t) = \zeta(t), \quad (4.1)$$

where dots denote time derivatives and $V'(q) = dV/dq$. The impact of the reservoir only appears through the friction rate γ and the stochastic force $\zeta(t)$, which has the properties

$$\langle \zeta(t) \rangle = 0, \quad \langle \zeta(t)\zeta(t') \rangle = 2m\gamma k_B T \delta(t - t') \quad (\text{white noise}).$$

This latter relation is known as a *fluctuation-dissipation theorem*, reflecting the fact that energy dissipation and stochastic scattering are inevitably connected since they have the same microscopic origin. A more realistic description takes into account the fact that the back-action of the reservoir on the system dynamics is time-retarded (colored noise), thus turning the constant friction rate into a time-dependent friction kernel $\gamma\dot{q}(t) \rightarrow \int_0^t ds \gamma(t-s)\dot{q}(s)$ (generalized Langevin equation). Anyway, the main message here is that, as long as we observe only the relevant particle, the impact of the reservoir is completely described by at least two macroscopic parameters, namely, the friction constant and the temperature, which can be determined experimentally. The complicated microscopic dynamics of the surrounding degrees of freedom need not be known.

4.3 Dissipative Quantum Systems

In contrast to the situation for classical systems, the inclusion of dissipation/fluctuations within quantum mechanics is much more complicated (Weiss 2008; Breuer and Petruccione 2002). A quantization of the classical Langevin Eq. (4.1) in terms of Heisenberg operators together with the quantum version of the fluctuation-dissipation theorem only applies for strictly linear dynamics (free particle, harmonic oscillator) and under the assumption that system and reservoir are initially independent. The crucial problem is that quantum mechanically the interaction between system and reservoir leads to a superposition of wave functions and thus to entanglement. This is easily seen when one assumes that the total compound system is described by a Hamiltonian of the form

$$H = H_S + H_I + H_R, \quad (4.2)$$

where a system H_S interacts via a coupling operator H_I with a thermal reservoir H_R . Whatever the structure of these operators, their pairwise commutators will certainly not all vanish. Typically, one has $[H_S, H_R] = 0$ while $[H_S, H_I] \neq [H_R, H_I] \neq 0$ for non-trivial dynamics to emerge. Accordingly, the operator for thermal equilibrium of the total structure, viz.,

$$W_\beta \sim \exp[-\beta(H_S + H_I + H_R)],$$

does not factorize (in contrast to the classical case). In a strict sense, the separation between the system and its environment no longer actually exists. Stating this in the context of the system-observer situation in quantum mechanics: the presence of an environment acts like an observer continuously probing the system dynamics.

The question is thus: how can we identify the system and reservoir from the full compound? The answer basically depends on the interests of the observer, and often simply on the devices available for preparation and measurement. Practically, one focuses on a set of observables $\{O_k\}$ associated with a specific sub-unit which in many cases coincides with the observables of a specific device that has been prepared or fabricated. The rest of the world remains unobserved. This then defines what is denoted as H_S in (4.2). Time dependent mean values follow from $\langle O_k \rangle = \text{Tr}_S\{O_k \rho(t)\}$, where the reduced density operator

$$\rho(t) = \text{Tr}_R\{U(t, 0)W(0)U(t, 0)^\dagger\} \quad (4.3)$$

is determined from the full time evolution $U(t, 0) = \exp(-iHt/\hbar)$ of an initial state $W(0)$ of the full compound by averaging over the unobserved reservoir degrees of freedom. Conceptually, this is in close analogy to the classical Langevin Eq. (4.1) on the level of a density operator, with the notable difference though that a consistent quantization procedure necessitates knowledge of a full Hamiltonian (4.2). For the system part this may be obvious, but it is in general extremely challenging, if not impossible, for the reservoir and its interaction with the system.

Progress is made by recalling that what we defined as the surroundings typically contains a macroscopic number of degrees of freedom and, since it is not directly prepared, manipulated, or detected, basically stays in thermal equilibrium (Weiss 2008). Large heat baths, however, display Gaussian fluctuations according to the central limit theorem. A very powerful description applying to a broad class of situations then assumes that a thermal environment consists of a quasi-continuum of independent harmonic oscillators linearly coupled to the system, i.e.,

$$H_R + H_I = \sum_k \frac{p_k^2}{2m_k} + \frac{m_k \omega_k^2}{2} \left(x_k - \frac{c_k}{m_k \omega_k^2} Q \right)^2. \quad (4.4)$$

Here Q denotes the operator of the system through which it is coupled to the bath (pointer variable). For systems with a continuous degree of freedom, it is typically given by the position operator (or a generalized position operator). The system-bath interaction is written in a translational invariant form so that the reservoir only affects the system dynamically in a similar way to what happens in the classical case (4.1). In fact, the classical version of this model reproduces the Langevin equation, implying that the influence of the reservoir on the system is completely determined by the temperature T and the spectral distribution of the bath oscillators, viz.,

$$J(\omega) = \frac{\pi}{2} \sum_k \frac{c_k^2}{2m_k \omega_k} \delta(\omega - \omega_k).$$

A continuous distribution $J(\omega)$ ensures that energy flow from the system into the bath occurs irreversibly (Poincaré's recurrence time tends to infinity). Each oscillator may only weakly interact with the system, but the effective impact of the collection of oscillators may still capture strong interaction. For instance, in the case of so-called Ohmic friction corresponding classically to white noise, one has $J(\omega) = m\gamma\omega$.

The bath force $\zeta = \sum_k c_k x_k$ acting on the system obeys Gaussian statistics and is thus completely determined via its first moment $\langle \zeta(t) \rangle = 0$ and its second moment $K(t) = \langle \zeta(t) \zeta(0) \rangle$. As an equilibrium correlation, it obeys the quantum fluctuation-dissipation theorem, namely,

$$\tilde{K}(\omega) = 2\hbar J(\omega) (1 - e^{-\omega\hbar\beta})^{-1}, \quad (4.5)$$

where $\tilde{K}(\omega)$ denotes the Fourier transform of $K(t)$ and $\beta = 1/k_B T$. One sees that for Ohmic dissipation $J(\omega) = m\gamma\omega$, and in the high temperature limit $\omega\hbar\beta \rightarrow 0$, the correlation becomes a constant $\tilde{K}(\omega) = 2m\gamma k_B T$ and thus describes the white noise known from classical dynamics (4.1). In the opposite limit of vanishing temperature $\omega\hbar\beta \rightarrow \infty$, however, one has $\tilde{K}(\omega) = 2m\gamma\hbar\omega$, which gives rise to an algebraic decay $K(t) \propto 1/t^2$. This non-locality in time reflects the discreteness of energy levels of reservoir oscillators and causes serious problems when evaluating the reduced dynamics. At low temperatures, the reduced quantum dynamics is always strongly retarded (non-Markovian) on time scales $\hbar\beta$, whence a simple time-local equation of motion does not generally exist. Equivalently, the idea of describing the time evolution of physical systems by means of equations of motion with suitable initial conditions is not directly applicable for quantum Brownian motion. It may hold approximately in certain limits such as very weak coupling (Breuer and Petruccione 2002) or, as we will see below, very strong dissipation.

The above procedure may also be understood from a different perspective. "What we observe as dissipation" in a system of interest is basically a consequence of our ignorance with respect to everything that surrounds this system. Dissipation is not inherent in nature, but rather follows from a concept that reduces the real

world to a small part to be observed and a much larger part to be left alone. In the sequel, we will illustrate the consequences of this reduction, which are much more subtle than in the classical domain.

4.4 Specific Heat for a Brownian Particle

According to conventional thermodynamics, the specific heat (for fixed volume) is given by

$$C_v = \frac{\partial U}{\partial T}, \quad (4.6)$$

where U denotes the internal energy of the system. Following classical concepts (Landau and Lifshitz 1958), the latter can be obtained either from the system energy (Hänggi et al. 2008)

$$\begin{aligned} U_E &= \langle H_S \rangle \\ &= \frac{\text{Tr}\{\exp(-\beta H) H_S\}}{\text{Tr}\{\exp(-\beta H)\}} \end{aligned} \quad (4.7)$$

or from the partition function

$$\begin{aligned} U_Z &= -\frac{\partial Z}{\partial \beta} \\ &= \frac{\text{Tr}\{\exp(-\beta H)\}}{\text{Tr}_R\{\exp(-\beta H_R)\}}. \end{aligned} \quad (4.8)$$

Here, we have used subscripts to distinguish between the two ways of obtaining the internal energy and thus the specific heat. Note that the partition function of the full compound system is defined with respect to the partition function of the bath alone. This is the only consistent way to introduce it, given that we average over the unobserved bath degrees of freedom. One easily realizes that the two routes may lead to quite different results, since

$$U_Z - U_E = \langle H_I \rangle + \langle H_R \rangle - \langle H_R \rangle_R. \quad (4.9)$$

Apart from the energy stored in the system-bath interaction, there also appears the difference in bath energies taken with respect to the full thermal distribution $\propto \exp(-\beta H)$ and the bath thermal distribution $\propto \exp(-\beta H_R)$. Classically, this difference vanishes due to the factorization of the thermal distribution. It may be negligible in the weak coupling regime where this factorization still holds approximately but certainly fails for stronger coupling and/or reservoirs with strongly non-Markovian behavior.

For a free quantum particle with so-called Drude damping, i.e., when $\gamma(t) = \gamma\omega_D \exp(-\omega_D t)$ or equivalently $J(\omega) = m\gamma\omega\omega_D/(\omega + \omega_D)$ with Drude frequency ω_D , one finds at low temperatures $T \rightarrow 0$ (Hänggi et al. 2008)

$$\frac{C_{v,E}}{k_B} \approx \frac{\pi k_B T}{3\hbar\gamma}, \quad \frac{C_{v,Z}}{k_B} \approx \frac{\pi k_B T}{3\hbar\gamma} \left(1 - \frac{\gamma}{\omega_D}\right), \quad (4.10)$$

in accordance with the third law of thermodynamics (vanishing specific heat for $T \rightarrow 0$). However, in contrast to $C_{v,E}$, the function $C_{v,Z}$ becomes negative for $\gamma/\omega_D > 1$, thus indicating a fundamental problem with this second way to obtain the specific heat. Apparently, the problem must be related to the definition (4.8) of the partition function of the reduced system. It does not exist in the high temperature regime or for Ohmic damping $\omega_D \rightarrow \infty$, and it is also absent for a harmonic system.

Any partition function can be expressed in terms of the density of states $\mu(E)$ of the system as $Z = \int_0^\infty dE \mu(E) \exp(-\beta E)$, which in turn allows us to retrieve $\mu(E)$ from a given partition function (Weiss 2008; Hänggi et al. 2008). Physically meaningful densities $\mu(E)$ must always be positive though. However, for reduced systems this is not the case in exactly those domains of parameter space where $C_{v,Z} < 0$. As a consequence, it only makes sense physically to start with the definition (4.7) for the specific heat, and this also implies that the partition function of a reduced quantum system does *not* play the same role as its counterpart in conventional classical thermodynamics.

This finding can once again be stated in the context of the measurement process in quantum physics: the expectation value of the system energy $\langle H_S \rangle$ is certainly experimentally accessible, while it seems completely unclear how to probe the partition function (4.8). One of its constituents, the partition function of the bare reservoir, cannot be measured as long as it is coupled to the system which, however, is not at the disposal of the experimentalist.

4.5 Roles Reversed: A Reservoir Dominates Coherent Dynamics

It is commonly expected that a noisy environment will tend to destroy quantum coherences in the system of interest and thus make it behave more classically. This gradual loss of quantumness has been of great interest recently because there has been a boost in activities to tailor atomic, molecular, and solid state structures with growing complexity and on growing length scales. A paradigmatic model is a two-state system interacting with a broadband heat bath of bosonic degrees of freedom (spin-boson model) which plays a fundamental role in a variety of applications (Weiss 2008; Breuer and Petruccione 2002; Leggett et al. 1987). Typically, at low temperatures and weak coupling, an initial non-equilibrium state evolves via damped coherent oscillations towards thermal equilibrium, while for stronger dissipation, relaxation occurs via an incoherent decay. This change from a quantum-type of

dynamics to a classical-type with increasing dissipation at fixed temperature (or with increasing temperature at fixed friction) is often understood as a quantum to classical transition. It has thus been analyzed in great detail to tackle questions about the validity of quantum mechanics on macroscopic scales or the appearance of a classical world from microscopic quantum mechanics.

However, the picture described above does not always apply, as has been found only very recently (Kast and Ankerhold 2013a, b). In particular, at least for a specific class of reservoir spectral densities, so-called sub-Ohmic spectral densities, the situation is more complex, with domains in parameter space where the quantum-classical transition is completely absent even for very strong dissipation. This persistence of quantum coherence corresponds to a strong system-reservoir entanglement, such that the dynamical properties of the two-level system are dominated by properties of the bath.

A generic example of a two-level system is a double-well potential where two energetically degenerate minima are separated by a high potential barrier (Weiss 2008; Leggett et al. 1987). At very low temperatures, only the degenerate ground states $|L\rangle$ and $|R\rangle$ in the left and the right well, respectively, are relevant. They are coupled via quantum tunneling through the potential barrier with a coupling energy $\hbar\Delta$. Hence, the corresponding Hamiltonian for this two-level system follows as $H_S = (\hbar\Delta/2)(|L\rangle\langle R| + |R\rangle\langle L|)$ and the interaction with the bath is mediated via the operator $Q \rightarrow (|L\rangle\langle L| - |R\rangle\langle R|)$ in (4.4). In this way, the reservoir tends to localize the system in one of the ground states, while quantum coherence tends to delocalize it (superpositions of $|L\rangle$ and $|R\rangle$). The competition between the two processes leads to a complex dynamics for the populations $\langle L|\rho(t)|L\rangle = 1 - \langle R|\rho(t)|R\rangle$ and in most cases to damped oscillatory motion (coherent dynamics) for weak and monotonic decay (classical relaxation) for strong friction.

Sub-Ohmic reservoirs appear in many condensed phase systems where low frequency fluctuations are more abundant than in standard Ohmic heat baths. The corresponding spectral function

$$J_s(\omega) = 2\pi\alpha\omega_c^{1-s}\omega^s, \quad 0 < s < 1, \quad (4.11)$$

depends on the spectral exponent s , a coupling strength α , and a frequency scale ω_c . In the limit $s \rightarrow 1$, one recovers the standard Ohmic distribution. In thermal equilibrium and at zero temperature, a two-level system embedded in such an environment displays two “phases”: a delocalized phase (quantum coherence prevails) for weaker friction and a localized phase (quantum non-locality destroyed) for stronger friction. The question then is: what does the relaxation dynamics towards these phases look like? The simple expectation is that the dynamics is quantum-like (oscillatory) in the former case and classical-like (monotonic decay) in the latter. That this is not always true is revealed by a numerical evaluation of (4.3).

As mentioned above, a treatment of the reduced quantum dynamics is a challenging task and, in fact, an issue of intense current research. While we refer to the literature [(Kast and Ankerhold 2013a, b) and references therein] for further details, we only mention that one powerful technique is based on the path integral

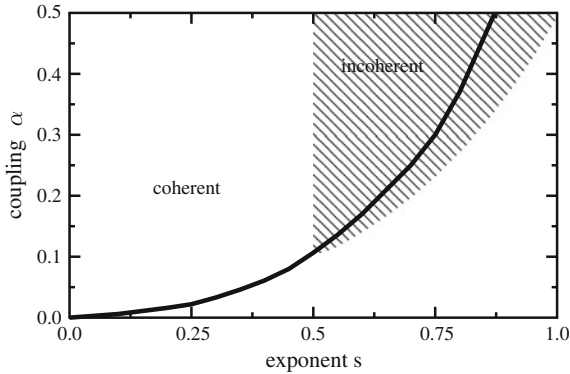


Fig. 4.1 Parameter space of a two-level system interacting with a sub-Ohmic reservoir with spectral exponent s and coupling strength α at $T = 0$. Below (above) the *black line*, for long times, the non-equilibrium dynamics approaches a thermal state with delocalized (localized) phase. This relaxation dynamics is incoherent only in the *shaded area* and coherent elsewhere, particularly, for $s < 1/2$ and also for strong friction

representation of (4.3) in combination with Monte Carlo algorithms. This numerical approach also allows one to access the strong friction regime in contrast to existing alternatives. As a result one gains a portrait in the parameter space of s, α (see Fig. 4.1) indicating the domains of coherent and incoherent non-equilibrium dynamics. Notably, for $0 < s < 1/2$, a transition from coherent to incoherent dynamics is absent even for strong coupling to the environment, and even though asymptotically the system approaches a thermal equilibrium with localized (classical-like) phase. It turns out that the frequency of this damped oscillatory population dynamics is given by $\Omega_s \approx 2\alpha\omega_c/s$ (for $s \ll 1$), with an effective damping rate $\gamma_0 \approx 2\alpha\omega_c$. Thus, the ratio $\Omega_s/\gamma_0 \approx 1/s \ll 1$, whence the system is strongly underdamped.

What is remarkable here is that these dynamical features of the two-level system are completely determined by properties of the reservoir. To leading order, the system energy scale $\hbar\Delta$ is negligible. In other words, on the one hand the system dynamics is slaved to the reservoir, and on the other hand the reservoir is no longer destructive but rather supports quantum coherent dynamics. This is only possible when system and bath are strongly entangled, which is indeed the case (Kast and Ankerhold 2013a). It is then at least questionable to consider the reservoir merely as a noisy background. Rather, in an experiment, one would access what are basically reservoir properties, whereas the two-level system acts only as a sort of mediator.

4.6 Emergence of Classicality in the Deep Quantum Regime

In conventional quantum thermodynamics one finds that, in the high temperature limit, classical thermodynamics is recovered. A simple example is a harmonic oscillator with frequency ω_0 . If the thermal scale $k_B T$ far exceeds the energy level

spacing $\hbar\omega_0$, quantization is washed out by thermal fluctuations and the oscillator displays classical behavior. For an open quantum system interacting with a real heat bath, an additional scale enters this scenario, namely, level broadening $\hbar\gamma$ (γ is a typical coupling rate) induced by the finite lifetime of energy eigenstates. In the weak coupling regime $\gamma \ll \omega_0$, the above argument then applies, and the classical domain is characterized by $\hbar\gamma \ll \hbar\omega_0 \ll k_B T$. Consequently, the scale $\hbar\gamma$ does not play any role and the classical Boltzmann distribution $\exp(-\beta H_S)$ does not depend on γ .

The same is true approximately at lower temperatures, where the canonical operator of the reduced system is given by that of the bare system, i.e., $\rho_\beta \propto \exp(-\beta H_S)$, as long as $\gamma \ll \omega_0$. In fact, even the reduced dynamics (4.2) can be cast into time-local evolution equations for the reduced density $\rho(t)$ if the time scale for bath-induced retardation $\hbar\beta$ is much shorter than the time scale for bath-induced relaxation $1/\gamma$. On a coarse-grained time scale, the reduced dynamics then appears to be Markovian. This domain

$$\frac{\hbar\gamma}{k_B T} \ll 1 \quad (4.12)$$

includes the weak friction regime $\gamma/\omega_0 \ll 1$, in which so-called master equations are valid down to very low temperatures $\hbar\omega_0/k_B T \gg 1$ (Breuer and Petruccione 2002) (see Fig. 4.2). It also contains the classical regime of strong friction $\gamma/\omega_0 \gg 1$ and very high temperatures $\omega_0 \hbar/k_B T \ll 1$. Anyway, in the domain defined via (4.12), the

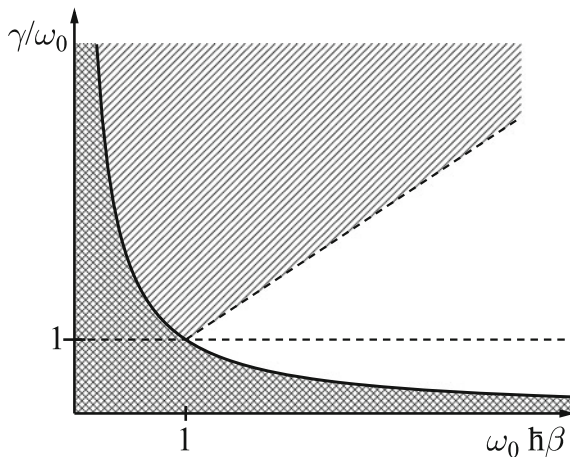


Fig. 4.2 Domains in parameter space for an open quantum system with typical energy level spacing $\hbar\omega_0$, interacting with a heat bath at reciprocal temperature β and with friction rate γ . Below the black line (grid shaded), the level broadening due to friction is negligible ($\gamma\hbar\beta \ll 1$), while above ($\gamma\hbar\beta \gg 1$), it must be treated non-perturbatively. The dashed horizontal line separates the domain of weak friction $\gamma/\omega_0 \ll 1$ from the overdamped one $\gamma/\omega_0 \gg 1$. At lower temperatures $\omega_0 \hbar\beta > 1$, classicality appears in the line-shaded domain where a time scale separation $\gamma/\omega_0^2 \gg \hbar\beta$ applies. See text for details

level broadening due to friction does not play a significant role and can be treated perturbatively.

The opposite is true for very strong dissipation $\gamma/\omega_0 \gg 1$ and low temperatures $\omega_0 \hbar/k_B T \gg 1$ (Ankerhold et al. 2001), so that

$$\frac{\hbar\gamma}{k_B T} \gg 1. \quad (4.13)$$

One might think that a simplification of the reduced dynamics is then not possible at all. However, it turns out that this is not quite true. Indeed, one must keep in mind that, in this regime, the relevant relaxation time scale for the reduced density is not given by $1/\gamma$, but rather by γ/ω_0^2 . This follows directly from the classical dynamics of the harmonic oscillator, whose two characteristic roots are given by

$$\lambda_{\pm} = -\frac{\gamma}{2} \pm \sqrt{\frac{\gamma^2}{4} - \omega_0^2}. \quad (4.14)$$

In the overdamped limit, the fast frequency $\lambda_- \approx \gamma$ corresponds to the fast equilibration of momentum, while the slow frequency $\lambda_+ \approx \omega_0^2/\gamma$ describes the much slower relaxation of position. Accordingly, on a coarse-grained time scale, one may consider the momentum part of the reduced density to be equilibrated to the instantaneous position, so that the position part is the only relevant quantity for the dynamics [note that the system interacts with the bath in (4.4) via the position operator].

This separation of time scales is well known in classical physics as the overdamped or Smoluchowski limit (Risken 1984). There, it corresponds to a reduction of the Langevin Eq. (4.1) in which inertia effects are adiabatically eliminated. Equivalently, the position part $P(q, t)$ of the full phase space distribution of a one-dimensional particle with mass m moving in a potential $V(q)$ obeys the famous Smoluchowski equation (Smoluchowski 1906; Risken 1984), a time evolution equation in the form of a diffusion equation

$$\frac{\partial P(q, t)}{\partial t} = \frac{1}{\gamma m} \frac{\partial}{\partial q} \left[V'(q) + k_B T \frac{\partial}{\partial q} \right] P(q, t). \quad (4.15)$$

For quantum Brownian motion one can indeed show (Ankerhold et al. 2001; Ankerhold 2007; Maier and Ankerhold 2010) that a generalization of this equation, the so-called quantum Smoluchowski equation, follows from the reduced dynamics (4.2) in the overdamped regime where $\gamma/\omega_0^2 \gg \hbar\beta$ (ω_0 then refers to a typical energy scale of the system, see Fig. 4.2). The diffusion constant has to be replaced by a position-dependent diffusion coefficient $D(q) = k_B T/[1 - \beta V''(q)\Lambda]$ according to $k_B T \partial/\partial q \rightarrow \partial/\partial q D(q)$. In the high temperature limit, one recovers the result (4.15) from $\Lambda \rightarrow 0$, while in the domain (4.13), one has $\Lambda \propto \ln(\gamma\hbar\beta)/\gamma$. Then, the dependence on the bath coupling γ and Planck's constant \hbar appears in a highly

non-perturbative way and may substantially influence the dynamics. However, the equation which governs this dynamics has a basically classical structure.

One may also understand the origin of an \hbar -dependent diffusion coefficient from Heisenberg's uncertainty relation. In the strong coupling regime, the reservoir squeezes fluctuations in position to the extent that the position distribution obeys a semi-classical type of equation of motion. This in turn requires momentum fluctuations to be strongly enhanced, which can indeed be shown. The quantum parameter Λ is reminiscent of this interdependence between position and momentum fluctuations. What is interesting experimentally, is the fact that, according to (4.13), quantum fluctuations may already appear at very high temperatures ($\hbar\omega_0 \ll k_B T$) if friction is sufficiently strong as, for example, in biological structures.

4.7 Summary and Conclusion

In this contribution we have shed some light on the subtleties that are associated with the description of open quantum systems. In contrast to the procedure in classical physics, quantum Brownian motion can only be consistently formulated when given a Hamiltonian of the full system. In a first step, this requires one to identify the relevant system part and its irrelevant surroundings, a choice which is not unique and depends on the focus of the observer. One then implements a reduction, keeping only the effective impact of the environment by assuming that it constitutes a heat bath. This has at least two substantial advantages: (i) a microscopic description of the actual reservoir is not necessary and (ii) this modeling provides a very general framework, applicable to a broad class of physical situations. In fact, it has turned out to be the most powerful approach we have for understanding experimental data for dissipative quantum dynamics. However, the price to pay for this reductionism is that, on the one hand, the dynamics cannot generally be cast into the form of simple time evolution equations, and on the other, conventional concepts and expectations must be treated with great caution.

The fundamental process is once again the non-locality of quantum mechanics, which in this context may lead to a "blurring" of what is taken to be the system and what is taken to be its surroundings. This entanglement becomes particularly serious when the interaction between the system and the heat bath is no longer weak. We have discussed here one example from thermodynamics and two examples from non-equilibrium dynamics. With respect to the first, it was shown that the partition function of a reduced system is not a proper partition function in the conventional sense and so cannot always be used to derive thermodynamic quantities. In the second and the third example, our naive conception of the division of the world into a classical realm and a quantum realm has been challenged. There may be emergence, with the consequence that quantum mechanics may survive even for strong friction and classicality may be found even in the deep quantum domain.

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