3
Quantum open systems

Before we develop the nonequilibrium aspects, we want to go over some basics of ordinary quantum mechanics [Dir58, LanLif76, Bes04]. Our goal is to review some formal manipulations which will be used later in the statistical physics contexts, and along the way establish some common notations. We shall develop the theory of quantum open systems from the point of view of the so-called Feynman–Vernon influence functional [FeyVer63, FeyHib65, CalLeg83a, GrScIn88, Kle90, HuPaZh92, HuPaZh93a, Wei93]. This approach and its closely related Schwinger–Keldysh or closed time path method will underlie the analysis of nonequilibrium quantum fields in the rest of the book. We refer the reader to the literature for alternative approaches to quantum open systems [GarZol00b, Car93, Per98].

3.1 A quick review of quantum mechanics

Let us consider a quantum mechanical system described by a single degree of freedom x. The states $|\alpha\rangle$ of the system live in a Hilbert space $\mathcal{H}$ and observables A are represented by Hermitian linear operators $\hat{A}$ in this space. We have different "pictures" of the dynamics, of which the most useful are the Schrödinger and Heisenberg ones. In the former, observables are time-independent, while states evolve in time according to the Schrödinger equation

$$i\hbar\frac{\partial}{\partial t}\left|\alpha\right\rangle = \hat{H}\left|\alpha\right\rangle \tag{3.1}$$

where the Hamiltonian operator $\hat{H}$ is associated with the observable "energy." This equation may be integrated

$$\left|\alpha\left(t\right)\right\rangle = U\left(t,t_0\right)\left|\alpha\left(t_0\right)\right\rangle, \tag{3.2}$$

with the evolution operator

$$U = T\left[\exp\left(-\frac{i}{\hbar}\int_{t_0}^{t} dt'\ \hat{H}\left(t'\right)\right)\right] \tag{3.3}$$

where T stands for temporal order. We are mostly interested in cases where the Hamiltonian is time-independent, whereby $U\left(t,t_0\right) = \exp\left(-i\hat{H}\left(t-t_0\right)/\hbar\right)$. In the Heisenberg picture states do not evolve, but observables do, according to the rule

$$\hat{A}\left(t\right) = U^{\dagger}\left(t\right)\hat{A}U\left(t\right) \tag{3.4}$$

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The rationale for this rule is that we get consistent values for expectation values of observables in either picture: $\left\langle \hat{A}(t) \right\rangle = \left\langle \alpha(t) \left| \hat{A}(0) \right| \alpha(t) \right\rangle_{\text{Sch}} = \left\langle \alpha(0) \left| \hat{A}(t) \right| \alpha(0) \right\rangle_{\text{Hei}}$. The evolution of operators in the Heisenberg picture is summarized by the Heisenberg equation

$$\frac{d\hat{A}}{dt} = \frac{i}{\hbar}\left[\hat{H}, \hat{A}\right] \tag{3.5}$$

As shown by Einstein, Podolsky and Rosen (EPR) [EiPoRo35], this quantum mechanical description of physical reality cannot be considered complete, since there are states of the system which are not described by kets in the Hilbert space. They occur when we know that the state of the system belongs with certainty to a given class of states $|\alpha_i\rangle$, but our knowledge does not allow us to go beyond assigning a probability of occurrence ρ_i to each member of this class. These situations are depicted by density matrices $\rho = \sum_i \rho_i |\alpha_i\rangle \langle\alpha_i|$, where we assume that the $|\alpha_i\rangle$ states are orthonormal. We always have $\text{Tr}\,\rho = 1$. Kets in the Hilbert space are particular cases of density matrices with $\text{Tr}\,\rho^2 = 1$, the general case being $\text{Tr}\,\rho^2 \leq 1$. In the Schrödinger picture, ρ is time-dependent, and obeys the Liouville–von Neumann equation

$$\frac{d\rho}{dt} = -\frac{i}{\hbar}\left[\hat{H}, \rho\right] \tag{3.6}$$

Observe that this is *not* the Heisenberg equation for the ρ matrix.

Let us now assume that the variable X is continuous and unbounded, and that the states $|x\rangle$ where this variable is well defined form a basis. We have the translation operators Π_a given by $\langle x| \Pi_a |\alpha\rangle = \langle x + a \mid \alpha\rangle$, which are unitary, and given the semigroup structure of these operators, we must have a Hermitian generator $\hat{P}$ such that $\Pi_a = \exp\left(ia\hat{P}/\hbar\right)$. The action of the generator is

$$\langle x| \hat{P} |\alpha\rangle = -i\hbar \frac{\partial}{\partial x} \langle x \mid \alpha\rangle \tag{3.7}$$

$\hat{P}$ has eigenstates $|p\rangle$ such that

$$\langle x \mid p\rangle = \frac{e^{ipx/\hbar}}{\sqrt{2\pi\hbar}} \tag{3.8}$$

The momentum observable $\hat{P}$ and the position observable $\hat{X}$ do not commute, but rather $\left[\hat{P}, \hat{X}\right] = -i\hbar\mathbf{1}$.

Consider a Hamiltonian of the form $\hat{H} = K(\hat{P}) + V(\hat{X})$, $K = \hat{P}^2/2M$. Since tK and tV do not commute, we cannot factor out the evolution operator as a product of a function of $\hat{P}$ times a function of $\hat{X}$. But since the commutator is of order t^2, factorization becomes a good approximation when t is small enough. This gives rise to the Trotter formula [Sch81]

$$e^{-it\hat{H}/\hbar} = \left[e^{-i\tau K/\hbar} e^{-i\tau V/\hbar}\right]^{N+1}, \qquad (N+1)\,\tau = t, \quad N \to \infty \tag{3.9}$$

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and thereby to the path integral representation of the evolution operator [FeyHib65, Sch81], since

$$\begin{aligned}\langle x_{N+1}|\,U(t)\,|x_0\rangle &= \langle x_{N+1}|\left[e^{-i\tau K/\hbar}e^{-i\tau V/\hbar}\right]^{N+1}|x_0\rangle \\ &= \int\left[\prod_{i=1}^{N}dx_i\right]\left\{\prod_{j=0}^{N}\langle x_{j+1}|\,e^{-i\tau K/\hbar}\,|x_j\rangle\,e^{-i\tau V(x_j)/\hbar}\right\} \\ &= \int\left[\prod_{i=1}^{N}dx_i\right]\left[\prod_{i=1}^{N+1}\frac{dp_i}{2\pi\hbar}\right] \\ &\quad\times\left\{\prod_{j=0}^{N}e^{ip_{j+1}(x_{j+1}-x_j)/\hbar}e^{-i\tau p_{j+1}^2/2M\hbar}e^{-i\tau V(x_j)/\hbar}\right\} \\ &= \int\left[\prod_{i=1}^{N}\sqrt{\frac{-iM}{2\pi\hbar\tau}}dx_i\right]\left\{\prod_{j=0}^{N}e^{iM(x_{j+1}-x_j)^2/2\tau\hbar}e^{-i\tau V(x_j)/\hbar}\right\}\end{aligned} \tag{3.10}$$

which as $N\to\infty$ yields

$$\langle x_t|\,U(t)\,|x_0\rangle = \int_{x(t)=x_t,x(0)=x_0} Dx\; e^{iS/\hbar} \tag{3.11}$$

The converse is also true, namely, if we take equation (3.11) as the definition of the evolution operator, we may derive the Schrödinger equation. We have

$$\langle x_t|\,U(t+\tau)\,|x_0\rangle = \int\sqrt{\frac{-iM}{2\pi\hbar\tau}}dx'\;e^{iM\left(x_t-x'\right)^2/2\tau\hbar}e^{-i\tau V\left(x'\right)/\hbar}\,\langle x'|\,U(t)\,|x_0\rangle \tag{3.12}$$

The Gaussian factor makes sure that only values $y\approx x_t$ contribute, so we may expand everything else in powers of $(y-x_t)$ and integrate term by term, whereby

$$\begin{aligned}\langle x_t|\,U(t+\tau)\,|x_0\rangle &= \left[1-\frac{i\tau}{\hbar}V(x_t)\right]\langle x_t|\,U(t)\,|x_0\rangle \\ &\quad+\frac{i\hbar\tau}{2M}\frac{\partial^2}{\partial x_t^2}\langle x_t|\,U(t)\,|x_0\rangle+O\left(\tau^2\right)\end{aligned} \tag{3.13}$$

QED

3.1.1 Wigner functions

So far, we have described states of a quantum system in terms of kets $|\alpha\rangle$ in a Hilbert space. Considering the position and momentum states $|x\rangle$ and $|p\rangle$, we may introduce the wavefunctions in position and momentum representations $\psi(x)=\langle x\mid\alpha\rangle$ and $\psi(p)=\langle p\mid\alpha\rangle$, which are related to each other through a Fourier transform

$$\psi(p)=\int\frac{dx}{\sqrt{2\pi\hbar}}\;e^{-ipx/\hbar}\psi(x) \tag{3.14}$$

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$|\psi(x)|^2$ and $|\psi(p)|^2$ represent the probability distribution functions for position and momentum, respectively. The question arises on whether these distributions may be obtained as marginal distributions from a joint probability for position and momentum. The answer is of course not, at least in general, since the existence of such a joint probability density would be almost conjured as saying that position and momentum may be simultaneously well defined. Nevertheless, in 1932 Wigner found an object which comes remarkably close [Wig32, HOSW84]. This object is the Wigner function

$$f^W(x,p) = \int \frac{du}{2\pi\hbar}\, e^{-ipu/\hbar}\psi^*\left(x-\frac{u}{2}\right)\psi\left(x+\frac{u}{2}\right) \tag{3.15}$$

Indeed, if we integrate over p we get the probability distribution for x

$$\int dp\, f^W(x,p) = |\psi(x)|^2 \tag{3.16}$$

while integrating over x and switching variables to $x \pm u/2$ we get

$$\int dx\, f^W(x,p) = |\psi(p)|^2 \tag{3.17}$$

The reason why f^W cannot be directly identified as a probability distribution function is that f^W, although real, is not necessarily nonnegative. We shall see examples below.

The dynamics of the Wigner function is also quite remarkable. If the wavefunction obeys the Schrödinger equation (equation (3.1) in the coordinate representation)

$$i\hbar\frac{\partial\psi}{\partial t} = -\frac{\hbar^2}{2M}\frac{\partial^2\psi}{\partial x^2} + V(x)\,\psi(x) \tag{3.18}$$

then

$$\begin{aligned}\frac{\partial f^W}{\partial t} &= \frac{1}{i\hbar}\int\frac{du}{2\pi\hbar}\, e^{-ipu/\hbar}\\ &\times\left\{\left(-\frac{\hbar^2}{2M}\right)\left[\psi^*\left(x-\frac{u}{2}\right)\frac{\partial^2\psi}{\partial x^2}\left(x+\frac{u}{2}\right)-\psi\left(x+\frac{u}{2}\right)\frac{\partial^2\psi^*}{\partial x^2}\left(x-\frac{u}{2}\right)\right]\right.\\ &\left.+\left[V\left(x+\frac{u}{2}\right)-V\left(x-\frac{u}{2}\right)\right]\psi^*\left(x-\frac{u}{2}\right)\psi\left(x+\frac{u}{2}\right)\right\}\end{aligned} \tag{3.19}$$

In the first line, we observe that

$$\begin{aligned}&\psi^*\left(x-\frac{u}{2}\right)\frac{\partial^2\psi}{\partial x^2}\left(x+\frac{u}{2}\right)-\psi\left(x+\frac{u}{2}\right)\frac{\partial^2\psi^*}{\partial x^2}\left(x-\frac{u}{2}\right)\\ &= 2\frac{\partial^2}{\partial u\partial x}\left[\psi^*\left(x-\frac{u}{2}\right)\psi\left(x+\frac{u}{2}\right)\right]\end{aligned}$$

After integration by parts, this term contributes

$$\frac{1}{i\hbar}\left(-\frac{\hbar^2}{2M}\right)\left(\frac{2ip}{\hbar}\right)\frac{\partial f^W}{\partial x} \equiv \frac{-p}{M}\frac{\partial f^W}{\partial x} \tag{3.20}$$

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The second term is much harder to handle. If the potential is smooth, one can try a Kramers–Moyal expansion [Kra40, Moy49, Kam81]

$$V\left(x+\frac{u}{2}\right)-V\left(x-\frac{u}{2}\right)=2\sum_{k=0}^{\infty}\frac{V^{(2k+1)}(x)}{(2k+1)!}\left(\frac{u}{2}\right)^{2k+1} \tag{3.21}$$

Commuting the integral and the sum, we obtain the second term as

$$\frac{2}{i\hbar}\sum_{k=0}^{\infty}\frac{V^{(2k+1)}(x)}{(2k+1)!}\left[\frac{i\hbar}{2}\frac{\partial}{\partial p}\right]^{2k+1}f^{W} \tag{3.22}$$

In terms of the classical Hamiltonian $H=p^2/2m+V$, our result reads

$$\frac{\partial f^{W}}{\partial t}=-\left\{H,f^{W}\right\}+O\left(\hbar^2\right) \tag{3.23}$$

where the Poisson bracket $\left\{H,f^{W}\right\}$ was introduced in Chapter 2, equation (2.48). In other words, the dynamics of the Wigner function follows remarkably closely the classical transport equation with external potential $V(x)$. If V is harmonic, there are no higher order terms, and the dynamics followed by the Wigner function is exactly the classical dynamics of a distribution function [Hab04, CDHR98]. However, as we have already remarked, that does not mean that f is classical, as it may be negative in some regions of phase space.

It is clear that we may compute the Wigner function f^{W} associated with any wavefunction ψ, but the converse is not true: it is easy to imagine phase space functions f^{W} which cannot be obtained as Wigner functions from *any* ψ. Indeed, it is enough to imagine a distribution function violating Heisenberg's uncertainty principle to exclude such an identification. To the best of our knowledge, there is no simple sufficient condition to see whether a given f^{W} is a Wigner function, although there are many necessary conditions (such as positivity of the marginal distributions).

To summarize, although f^{W} itself cannot be understood as a probability density, conveniently smeared versions of f^{W} are nonnegative and may be used to assign probabilities to different events. This restricted interpretation of the Wigner function will be enough for our requirements below.

Some examples

The simplest possible example of a Wigner function is a momentum state

$$\psi(x)=\frac{e^{i\mathbf{p}x/\hbar}}{\sqrt{2\pi\hbar}} \tag{3.24}$$

Then

$$f^{W}=\frac{1}{2\pi\hbar}\delta(p-\mathbf{p}) \tag{3.25}$$

Now consider a stationary wave

$$\psi(x)=\frac{1}{\sqrt{\pi\hbar}}\cos\left(\frac{\mathbf{p}x}{\hbar}\right) \tag{3.26}$$

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representing a coherent superposition of two states of opposite momentum. Then

$$f^W(x,p) = \frac{1}{4\pi\hbar}\left[\delta(p-\mathbf{p}) + \delta(p+\mathbf{p})\right] + \cos\left(\frac{2\mathbf{p}x}{\hbar}\right)\delta(p) \tag{3.27}$$

We see that f^W is not nonnegative. The oscillatory terms are related to the interference between the two components of the wave packet [PaHaZu93].

As a second example, let us consider a Gaussian wave packet

$$\psi(x) = \frac{e^{-x^2/4\sigma^2}}{(2\pi\sigma^2)^{1/4}} \tag{3.28}$$

Then

$$f^W(x,p) = \frac{1}{\pi\hbar}e^{-x^2/2\sigma^2}e^{-2\sigma^2(p/\hbar)^2} \tag{3.29}$$

In this case f^W is positive definite, and the dispersions in x and p are what may be expected for a minimum uncertainty state.

In particular, suppose our state is the ground state for a harmonic oscillator. Then $\sigma^2 = \hbar/2M\Omega$, and

$$f^W(x,p) = \frac{1}{\pi\hbar}\exp\left\{-\frac{E}{\varepsilon}\right\}; \qquad \varepsilon = \frac{1}{2}\hbar\Omega,\ E = \frac{p^2}{2M} + \frac{M\Omega^2x^2}{2} \tag{3.30}$$

As a final example, let us consider a superposition of two Gaussian wave packets

$$\psi(x) = \frac{1}{(2\pi\sigma^2)^{1/4}}\left\{Ae^{-(x-a)^2/4\sigma^2} + Be^{-(x+a)^2/4\sigma^2}\right\} \tag{3.31}$$

leading to

$$\begin{aligned} f^W(x,p) = \frac{e^{-2\sigma^2(p/\hbar)^2}}{\pi\hbar}\Big\{&|A|^2 e^{-(x-a)^2/2\sigma^2} + |B|^2 e^{-(x+a)^2/2\sigma^2} \\ &+ e^{-x^2/2\sigma^2}\left[AB^*e^{-2ipa/\hbar} + A^*Be^{2ipa/\hbar}\right]\Big\} \end{aligned} \tag{3.32}$$

Again, we see nonpositive terms arising from the interference between the different components. If A and B had random phases, f^W would be nonnegative.

Wigner functions and probabilities

We know that if the system is in the state $\psi(x)$, the probability of observing it in the state $\phi(x)$ is

$$P = \left|\int dx\ \phi^*(x)\,\psi(x)\right|^2 \tag{3.33}$$

If we call f^W_ψ and f^W_ϕ the corresponding Wigner functions, and call

$$Q = 2\pi\hbar\int dxdp\ f^W_\psi(x,p)\,f^W_\phi(x,p) \tag{3.34}$$

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then $P = Q$. Indeed

$$\begin{aligned} Q &= \int dxdp \int \frac{dudu'}{2\pi\hbar}\, e^{-ip(u+u')/\hbar}\psi^*\left(x-\frac{u}{2}\right) \\ &\quad \times\psi\left(x+\frac{u}{2}\right)\phi^*\left(x-\frac{u'}{2}\right)\phi\left(x+\frac{u'}{2}\right) \\ &= \int dxdu\, \psi^*\left(x-\frac{u}{2}\right)\psi\left(x+\frac{u}{2}\right)\phi^*\left(x+\frac{u}{2}\right)\phi\left(x-\frac{u}{2}\right) = P \end{aligned} \tag{3.35}$$

This implies in particular that the inner product (3.34) of two Wigner functions must be positive. Since Gaussian distributions consistent with Heisenberg's principle are allowed Wigner functions, this implies that Gaussian smearings of a Wigner function are positive definite.

3.1.2 Closed time path (CTP) integrals

Recall that states evolve according to equation (3.2). Using the matrix elements (3.11) for the evolution operator, we obtain

$$\psi(x,t) = \int dx(0)\; U(x,x(0),t)\,\psi(x(0),0) = \int_{x(t)=x} Dx\; e^{iS/\hbar}\psi(x(0),0) \tag{3.36}$$

in the coordinate representation, where $U(x,x(0),t) = \langle x|\,U(t)\,|x(0)\rangle$. By linearity, we infer that the density matrix evolves according to

$$\begin{aligned} \rho(x,x',t) &= \langle x|\,U(t)\,\rho U^\dagger(t)\,|x'\rangle \\ &= \int_{x(t)=x,x'(t)=x'} DxDx'\; e^{i\left(S[x]-S\left[x'\right]\right)/\hbar}\rho(x(0),x'(0),0) \end{aligned} \tag{3.37}$$

The possibility of cyclic permutations under a trace shows that $\mathrm{Tr}\,\rho(t) = \mathrm{Tr}\,\rho(0) = 1$, as it should.

We see that the path integral representation involves *two* histories, rather than a single history of the system as in equation (3.11). This observation is the departure point of the so-called closed time path formalism, which we shall develop at length in this book, especially in Chapters 5 and 6; for source references see [Sch60, Sch61, BakMah63, Kel64, ChoSuHa80, CSHY85, SCYC88, DeW86, Jor86, CalHu87, CalHu88, CalHu89]. To investigate further the meaning of these two-time-path integrals, let us consider the expression

$$G^{11}(\tau,\tau') = \int_{x(t)=x'(t)} DxDx'\; e^{i\left(S[x]-S\left[x'\right]\right)/\hbar}\rho(x(0),x'(0),0)\;\; x(\tau)\,x(\tau') \tag{3.38}$$

The upper limit is free, provided it is the same for both histories. We may describe this as an integral over single histories defined on a *closed time path* (CTP). This time path has a first branch from 0 to t, where the history takes the values $x(t)$,

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and a second branch from t back to 0, where the history takes the values $x'(t)$. The CTP boundary condition $x(t) = x'(t)$ says that the history is continuous as a function on the time path.

To understand why we are describing the second branch as going backwards in time, let us translate $G^{11}(\tau, \tau')$ to canonical language. To this end, let us assume $\tau > \tau'$, and make explicit the value of the histories at these two preferred times, namely

$$\begin{aligned} G^{11}(\tau, \tau') = \int & dx(0)\, dx'(0)\;\; dx(\tau')\, dx(\tau)\, dx(t) \\ & \times \left[\int_{0 \le t \le \tau'} Dx\; e^{iS[x]/\hbar}\right] x(\tau') \left[\int_{\tau' \le t \le \tau} Dx\; e^{iS[x]/\hbar}\right] x(\tau) \\ & \times \left[\int_{\tau \le t \le t} Dx\; e^{iS[x]/\hbar}\right] \left[\int_{x'(t)=x(t)} Dx'\; e^{-iS\left[x'\right]/\hbar}\right] \\ & \times \rho(x(0), x'(0), 0) \end{aligned} \tag{3.39}$$

Identifying each bracket as a matrix element for some evolution operator, we get

$$\begin{aligned} G^{11}(\tau, \tau') = \int & dx(0)\, dx'(0)\;\; dx(\tau')\, dx(\tau)\, dx(t) \\ & \times \langle x(t)|\, U(t, \tau)\, |x(\tau)\rangle\;\; x(\tau)\;\; \langle x(\tau)|\, U(\tau, \tau')\, |x(\tau')\rangle\;\; x(\tau') \\ & \times \langle x(\tau')|\, U(\tau', 0)\, |x(0)\rangle\;\; \langle x(0)|\, \rho\, |x'(0)\rangle\;\; \langle x'(0)|\, U(0, t)\, |x(t)\rangle \\ = & \; Tr\; \left\{U(t, \tau)\;\hat{X}\, U(\tau, \tau')\;\hat{X}\, U(\tau', 0)\;\rho(0)\;U(0, t)\right\} \end{aligned} \tag{3.40}$$

in the Schrödinger representation, or equivalently

$$G^{11}(\tau, \tau') = Tr\; \left\{\hat{X}(\tau)\, \hat{X}(\tau')\, \rho\right\} \equiv \left\langle \hat{X}(\tau)\, \hat{X}(\tau')\right\rangle \tag{3.41}$$

in the Heisenberg representation. Observe that if we had not specified the relationship between τ and τ', then the path integral would have automatically set the largest time to the left. This expresses the "time ordering" of the two Heisenberg operators, so that we may generalize the result to $G^{11}(\tau, \tau') \equiv \left\langle T\left[\hat{X}(\tau)\, \hat{X}(\tau')\right]\right\rangle$, where T stands for temporal ordering.

Now consider instead

$$G^{12}(\tau, \tau') = \int_{x(t)=x'(t)} Dx Dx'\; e^{i\left(S[x]-S\left[x'\right]\right)/\hbar} \rho(x(0), x'(0), 0)\;\; x(\tau)\, x'(\tau') \tag{3.42}$$

The corresponding Schrödinger picture canonical expression is

$$G^{12}(\tau, \tau') = Tr\; \left\{U(0, \tau')\;\hat{X}\, U(\tau', t)\;U(t, \tau)\;\hat{X}\, U(\tau, 0)\;\rho(0)\right\} \tag{3.43}$$

or, in Heisenberg's representation, $G^{12}(\tau, \tau') \equiv \left\langle \hat{X}(\tau')\, \hat{X}(\tau)\right\rangle$. In this case, the primed Heisenberg operator comes out to the left, whichever time is greatest. We may think of this as a *path*, rather than a time, ordering. Finally, with the

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same argument we see that

$$G^{22}(\tau,\tau') = \int_{x(t)=x'(t)} DxDx'\, e^{i\left(S[x]-S\left[x'\right]\right)/\hbar}\rho\left(x\left(0\right),x'\left(0\right),0\right)\ \left\{x'\left(\tau\right)x'\left(\tau'\right)\right\}$$
$$\equiv \left\langle \tilde{T}\left[\hat{X}\left(\tau\right)\hat{X}\left(\tau'\right)\right]\right\rangle \tag{3.44}$$

where $\tilde{T}$ stands for *anti*-time ordering (that is, the latest time to the right). This anti-time ordering property justifies regarding the second branch as going backwards with respect to the first branch.

If necessary, more involved time paths may be considered. For example, it may be that the initial density matrix corresponds to a thermal state $\rho(0) = e^{-\beta H}/Z$, which can be regarded as an evolution operator in Euclidean time $\tau_\beta = -i\hbar\beta$. Then its matrix elements admit a path integral representation on a time branch going from 0 to τ_β, which appears as a third branch in the path integral representation for average values [Mil69, McL72a, McL72b]. We will have a lot more to say on thermal states in Chapter 10.

3.2 Influence functional

We wish to use the above to study the dynamics of a quantum open system. The set-up is the usual one: a system S described by a variable x interacts with an environment E described by variable(s) $q = \{q_n\}$. The classical action takes the form $S[x,q] = S_S[x] + S_E[q] + S_{\text{int}}[x,q]$. The Hamiltonian $\hat{H} = \hat{H}_S + \hat{H}_E + \hat{H}_{\text{int}}$, where

$$\hat{H}_s = \frac{1}{2}p^2 + V(x)\,; \qquad \hat{H}_{\text{int}} = V_{\text{int}}(x,q) \tag{3.45}$$

The quantum state of the total system is described by the density matrix $\rho(xq,x'q',t)$ depending on both system and environment variables. It evolves unitarily under $\hat{H}$ from an initial density matrix $\rho(0)$ at $t=0$ to $\rho(t) = e^{-it\hat{H}/\hbar}\rho(0)\,e^{it\hat{H}/\hbar}$ at finite time t. Explicitly, using completeness conditions in a path integral representation:

$$\begin{aligned}
\rho(x\,q,\,x'\,q,\,t) &= \langle x\,q,\,t|\rho|x'\,q,\,t\rangle \\
&= \int dx_i\,dq_i \int dx_i'\,dq_i'\ \langle x\,q,\,t|x_i\,q_i,\,0\rangle\langle x_i\,q_i,\,0|\rho|x_i'\,q_i',0\rangle\langle x_i'\,q_i',\,0|x'\,q,t\rangle \\
&= \int dx_i\,dq_i \int dx_i'\,dq_i' \int_{x_i}^{x} Dx \int_{q_i}^{q} Dq\ e^{iS[x,q]/\hbar}\rho(x_i\,q_i,\,x_i'\,q_i',\,0) \\
&\quad \times \int_{x_i'}^{x'} Dx' \int_{q_i'}^{q} Dq'\ e^{-iS[x',q']/\hbar} \\
&\equiv \int dx_i\,dq_i \int dx_i'\,dq_i'\ \mathcal{J}(x\,q,\,x'\,q,\,t|x_i\,q_i,\,x_i'\,q_i',\,0)\ \rho(x_i\,q_i,\,x_i'\,q_i',\,0)
\end{aligned} \tag{3.46}$$

where $\mathcal{J}$ is seen to be an evolution operator for the system plus environment.

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Since we care more about the system's behavior than the environment, we need not keep track of the details of the environment in the specifics of its Hamiltonian. In particular, we are mostly interested in computing the expectation values of system observables. Considered as operators on the whole Hilbert space for the system, these take the form $\hat{A} \otimes \mathbf{1}$, where $\hat{A}$ is an operator in the system Hilbert space, and $\mathbf{1}$ is the unit operator on the environment Hilbert space. The expectation value of such observables may be computed with the *reduced* density matrix ρ_r. This is obtained from the total density matrix as a partial (Landau's) trace over the environment variables, namely $\rho_r = \mathrm{Tr}_q\, \rho$. Explicitly,

$$\rho_r(x\, x',\, t) = \int_{-\infty}^{\infty} dq\; \rho(x\, q,\, x'\, q,\, t) \tag{3.47}$$

Let us further assume that at $t = 0$ the system and environment (variables with subscript i) are uncorrelated,

$$\rho(x_i\, q_i,\, x_i'\, q_i',\, 0) = \rho_S(x_i\, x_i',\, 0)\; \rho_E(q_i\, q_i',\, 0) \tag{3.48}$$

(Thus we are bringing the system and its environment together with all due care to avoid the complications associated with the sudden switching on and off of interactions. For the general case, see [HakAmb85, MorCal87, DavPaz97].) As such, we are able to rearrange the order of integration to write the reduced density matrix in the following way:

$$\rho_r(x\, x',\, t) = \int dx_i\, dx_i'\; \mathcal{J}_r(x\, x',\, t|x_i\, x_i',\, 0)\; \rho_S(x_i\, x_i',\, 0) \tag{3.49}$$

where the evolution operator for the reduced density matrix is defined by

$$\mathcal{J}_r(x\, x',\, t|x_i\, x_i',\, 0) \equiv \int_{x_i}^{x} Dx \int_{x_i'}^{x'} Dx'\; e^{i\hbar^{-1}\left(S[x]-S[x']\right)}\; \mathcal{F}[x, x'] \tag{3.50}$$

$\mathcal{F}[x, x']$ is the so-called Feynman–Vernon influence functional [FeyVer63, FeyHib65, Wei93]:

$$\begin{aligned}\mathcal{F}[x, x'] &\equiv e^{iS_{\mathrm{IF}}[x,x',t]/\hbar} \\ &= \int dq\; dq_i\; dq_i'\; \rho_E(q_i\, q_i'\, 0) \int_{q_i}^{q} Dq\; e^{i\hbar^{-1}(S_E[q]+S_{int}[x,q])} \\ &\quad \times \int_{q_i'}^{q} Dq'\; e^{-i\hbar^{-1}\left(S_E[q']+S_{int}[x',q']\right)}\end{aligned} \tag{3.51}$$

Here, S_{IF} is called the influence action. Equation (3.49) looks like the evolution of a density matrix for a closed system, but it contains a nonlocal term S_{IF}, which induces an explicit interaction between the two histories in the CTP. All the influence of the environment on the system is encoded into the influence action S_{IF}.

We can also write the influence functional in a basis-independent form as follows. In terms of the propagators $U(t), U'(t)$ for $S_E[q] + S_{\mathrm{int}}[x, q]$ and

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$S_E[q] + S_{\rm int}[x', q]$, respectively, the path integrals can be expressed as

$$\mathcal{F}[x, x'] = \int dq\, dq_i\, dq_i'\, \rho_E(q_i\, q_i',\, 0)\, \langle q|U(t)|q_i\rangle\, \langle q_i'|U'^{\dagger}(t)|q\rangle \tag{3.52}$$

Then upon integrating over q, q_i and writing the remaining integral as a trace, we obtain:

$$\mathcal{F}[x, x'] = \mathrm{Tr}\, U(t)\, \rho_E(0)\, U'^{\dagger}(t) \tag{3.53}$$

3.2.1 Some properties of the influence action

Let us explore the main properties of the influence action. From equation (3.53)

$$e^{iS_{\rm IF}\left[x,x',t\right]/\hbar} = \mathrm{Tr}\ \{U_{x'}\,(0,t)\, U_x\,(t,0)\, \rho_E\,(0)\} \tag{3.54}$$

The U's represent evolution operators with respect to a dynamics where the system variable x plays the role of an external, time-dependent parameter. For two different histories $x\,(t)$ and $x'\,(t)$ the U's do not cancel each other. But when $x = x'$, they do, and we get $S_{\rm IF}\,[x, x, t] \equiv 0$. Even in the presence of an explicit time dependence, the evolution operator U_x is unitary, whereby $S_{\rm IF}\,[x', x, t] \equiv -S_{\rm IF}\,[x, x', t]^*$. This means that, in a functional Taylor expansion in terms of the difference variable $u = x - x'$ and the "center of mass" variable $X = (x + x')\,/2$,

$$S_{\rm IF}\,[X, u, t] = \sum_{k=1} \frac{1}{k!} \int dt_1 \ldots dt_k\, S^{(k)}\,[X\,(\tau)\,, t_1, \ldots t_k, t]\, u\,(t_1) \ldots u\,(t_k) \tag{3.55}$$

all the odd terms are real, and all the even terms are imaginary. Taking a variation along the diagonal we get the additional property $S_{{\rm IF},x}\big|_{x=x'} = -\, S_{{\rm IF},x'}\big|_{x=x'}$.

At this point, it is convenient to introduce a notation that will stay with us for the rest of the book. Let us call $x\,(t) = x^1\,(t)$, $x'\,(t) = x^2\,(t)$. We shall think of x^a, $a = 1, 2$, as a single field doublet defined on a conventional (single branch) time path. Moreover, as in a σ model, we define a metric tensor $c_{ab} = \mathrm{diag}(1, -1)$ in target space. The metric tensor, together with its contravariant $(c^{ab} = (c^{-1})^{ab} = \mathrm{diag}\,(1, -1))$ and mixed $(c^a_b = c^{ad} c_{db} = \delta^a_b)$ forms may be used to raise and/or lower indices, as in $x_1 = c_{1a} x^a = x^1 = x$, $x_2 = c_{2a} x^a = -x^2 = -x'$. From now on, the Einstein convention of summation over repeated indices will be assumed; for example, the kinetic terms in the system action will be written as

$$\frac{1}{2} \int dt\, c_{ab} \dot{x}^a \dot{x}^b = \frac{1}{2} \int dt\, \dot{x}_a \dot{x}^a = \frac{1}{2} \int dt\ \left[\dot{x}^2 - \dot{x}'^2\right] \tag{3.56}$$

and we shall refer to the *CTP action* $S\,[x^a] \equiv S\,[x] - S\,[x']$ without discriminating the contributions from either branch.

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3.2.2 The linear bath model

As an example, let us assume that the environment action is quadratic in the (many) q variable(s), the initial environment density matrix is Gaussian, and the interaction term is bilinear $S_{\rm int} = \int dt\, x^a(t)\, Q_a[q(t)]$ (in CTP notation!), where the Q's are linear combinations of the q's [CalLeg83a, CalLeg83b, GrScIn88]. Under all these assumptions, the influence action must also be quadratic in x and x' (equation (3.51) is a functional Fourier transform of an elaborate Gaussian functional of histories $Q(t)$ and $Q'(t)$, and the Fourier transform of a Gaussian is another Gaussian). Therefore we write $S_{\rm IF} = (1/2)\int dtdt'\, x^a(t)\, \mathbf{M}_{ab}(t,t')\, x^b(t')$, where

$$\mathbf{M}_{ab}(t,t') = -i\hbar\, \frac{\delta^2}{\delta x^a(t)\,\delta x^b(t')} e^{iS_{\rm IF}[x^a,T]/\hbar}\bigg|_{x^a=0} \tag{3.57}$$

A direct variation from equation (3.51) yields

$$\begin{aligned}\frac{\delta^2 e^{iS_{\rm IF}[x^a,T]/\hbar}}{\delta x^a(t)\,\delta x^b(t')}\bigg|_{x^a=0} &= \frac{-1}{\hbar^2}\int_{q^1(T)=q^2(T)} Dq^a\; e^{iS_E[q^a]/\hbar} Q_a(t) \\ &\quad \times Q_b(t')\,\rho_e\left(q^1(0), q^2(0), 0\right)\end{aligned} \tag{3.58}$$

As per the earlier discussion, we obtain

$$\mathbf{M}_{ab}(t,t') = \frac{i}{\hbar}\begin{pmatrix} \langle T[Q(t)\,Q(t')]\rangle & -\langle Q(t')\,Q(t)\rangle \\ -\langle Q(t)\,Q(t')\rangle & \left\langle \tilde{T}[Q(t)\,Q(t')]\right\rangle \end{pmatrix} \tag{3.59}$$

(where the expectation values are computed *disregarding* the interaction with the system), or, in terms of the original variables

$$\begin{aligned}S_{\rm IF} = \frac{i}{2\hbar}\int dtdt' \Big\{&\langle T[Q(t)\,Q(t')]\rangle\, x(t)\,x(t') - \langle Q(t')\,Q(t)\rangle\, x(t)\,x'(t') \\ &- \langle Q(t)\,Q(t')\rangle\, x'(t)\,x(t') + \left\langle \tilde{T}[Q(t)\,Q(t')]\right\rangle x'(t)\,x'(t')\Big\}\end{aligned} \tag{3.60}$$

If we now write $x = X + u/2$, $x' = X - u/2$, we get the equivalent expression

$$S_{\rm IF} = \int dtdt' \left\{u(t)\,\mathbf{D}(t,t')\,X(t') + \frac{i}{2}\,u(t)\,\mathbf{N}(t,t')\,u(t')\right\} \tag{3.61}$$

where we encounter for the first time the *dissipation* $\mathbf{D}$ and *noise* $\mathbf{N}$ kernels

$$\mathbf{D}(t,t') = \frac{i}{\hbar}\langle[Q(t), Q(t')]\rangle\,\theta(t-t'); \qquad \mathbf{N}(t,t') = \frac{1}{2\hbar}\langle\{Q(t), Q(t')\}\rangle \tag{3.62}$$

Square and curly brackets stand for commutator and anticommutator, respectively. They are both real, as expected, and $\mathbf{D}$ is also causal.

Unraveling the physical meaning of these kernels and applying them to different situations will be a major theme for the rest of the book.

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3.3 The master equation

When the influence functional is quadratic, and hence may be written as in equation (3.61), it is possible to derive a dynamical equation for the evolution of the reduced density matrix [Zha90, HuPaZh92, HuPaZh93a, PaHaZu93, Paz94, HalYu96].

First use equation (3.61), plus the observation that $\mathbf{D}$ is causal and vanishes on the diagonal (cf. equation (3.62)), to obtain an explicit representation for $S_{\mathrm{IF}}[t+dt]$

$$S_{\mathrm{IF}}[x^a, t+dt] = S_{\mathrm{IF}}[x^a, t] + dt\, u(t) \int_0^t dt' \; \{\mathbf{D}(t,t')\, X(t') + i\mathbf{N}(t,t')\, u(t')\} \tag{3.63}$$

Now use this in equation (3.49) to obtain

$$\begin{aligned} \frac{\partial}{\partial t}\rho_r(x,x',t) = &-\frac{i}{\hbar}\left[\hat{H}_s, \rho_r(t)\right]_{x,x'} \\ &-\frac{1}{\hbar}(x-x')\int_0^t dt' \left\{\mathbf{N}(t,t')\left[\mathbf{X}-\mathbf{X}'\right](x,x',t')\right. \\ &\left.-\frac{i}{2}\mathbf{D}(t,t')\left[\mathbf{X}+\mathbf{X}'\right](x,x',t')\right\} \end{aligned} \tag{3.64}$$

The first term is just the Liouville–von Neuman equation (3.6) for the closed system. In the second term

$$\begin{aligned} \mathbf{X}(x,x',t') = &\int_{x(t)=x, x'(t)=x'} DxDx' \; e^{i(S_S[x]-S_S[x']+S_{\mathrm{IF}}[x,x',t])/\hbar} \\ &\times \rho_s(x(0), x'(0), 0) \; x(t') \end{aligned} \tag{3.65}$$

with a similar expression for $\mathbf{X}'(x,x',t')$, replacing the last factor $x(t')$ by $x'(t')$.

In general, $\mathbf{X}(x,x',t')$ and $\mathbf{X}'(x,x',t')$ are complicated functions of x, x' and t. However, since in general $\mathbf{N}$ and $\mathbf{D}$ are of second order in the system–bath interaction (cf. equation (3.62)), S_{IF} may be neglected within the integral in equation (3.65) to third order in this interaction, and $\mathbf{X}(x,x',t')$ and $\mathbf{X}'(x,x',t')$ may be expressed in terms of quantities belonging to the system alone. Concretely, $\mathbf{X}(x,x',t')$ is the (x,x') matrix element of the operator

$$\mathbf{X}(t') = e^{-i\hat{H}_s(t-t')/\hbar}\hat{X}e^{-i\hat{H}_s t'/\hbar}\rho_s(0)\, e^{i\hat{H}_s t/\hbar} \tag{3.66}$$

where $\hat{X}$ is the position operator in the Schrödinger representation. Introducing the Heisenberg operator $\hat{X}(t) = e^{i\hat{H}_s t/\hbar}\hat{X}e^{-i\hat{H}_s t/\hbar}$ and writing $t' = t-\tau$, we get, to second order in the system–bath coupling

$$\mathbf{X}(t') = \hat{X}(-\tau)\,\rho_r(t) \tag{3.67}$$

Similarly, $\mathbf{X}'(x,x',t')$ is the (x,x') matrix element of the operator

$$\mathbf{X}'(t') = \rho_r(t)\,\hat{X}(-\tau) \tag{3.68}$$

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whereby we get the so-called master equation

$$\begin{aligned}\hbar\frac{\partial}{\partial t}\rho_r(t) = &-i\left[H_s, \rho_r(t)\right] \\ &-\int_0^t d\tau \left\{\mathbf{N}(t, t-\tau)\left[\hat{X}, \left[\hat{X}(-\tau), \rho_r(t)\right]\right]\right. \\ &\left.-\frac{i}{2}\mathbf{D}(t, t-\tau)\left[\hat{X}, \left\{\hat{X}(-\tau), \rho_r(t)\right\}\right]\right\} \end{aligned} \tag{3.69}$$

3.3.1 The linear system model

When the system is also linear we can give an explicit formula for the Heisenberg operators

$$\hat{X}(-\tau) = \cos[\Omega\tau]\ \hat{X} - \frac{\sin[\Omega\tau]}{M\Omega}\ \hat{P} \tag{3.70}$$

and we can write the master equation in a way which is explicitly local in time

$$\begin{aligned}\hbar\frac{\partial}{\partial t}\rho_r(x, x', t) = &\left\{\frac{i\hbar^2}{2M}\left[\frac{\partial^2}{\partial x^2} - \frac{\partial^2}{\partial x'^2}\right] - \frac{iM\left[\Omega^2 + \delta\Omega^2(t)\right]}{2}\left(x^2 - x'^2\right)\right. \\ &-\frac{\sigma^2(t)}{2\hbar}(x - x')^2 - i\Delta_{ad}(t)(x - x')\left[\frac{\partial}{\partial x} + \frac{\partial}{\partial x'}\right] \\ &\left.-\hbar\Gamma(t)(x - x')\left[\frac{\partial}{\partial x} - \frac{\partial}{\partial x'}\right]\right\}\rho_r(x, x', t) \end{aligned} \tag{3.71}$$

where

$$\frac{\sigma^2(t)}{2} = \int_0^t d\tau\ \hbar\mathbf{N}(t, t-\tau)\cos[\Omega\tau] \tag{3.72}$$

$$\Delta_{ad}(t) = \frac{1}{M\Omega}\int_0^t d\tau\ \hbar\mathbf{N}(t, t-\tau)\sin[\Omega\tau] \tag{3.73}$$

$$\Gamma(t) = \frac{1}{2}\int_0^t d\tau\ \gamma(\tau)\cos[\Omega\tau] \tag{3.74}$$

$$\delta\Omega^2(t) = \Omega\int_0^t d\tau\ \gamma(\tau)\sin[\Omega\tau] - \gamma(0) \tag{3.75}$$

and we have written $\mathbf{D}(t, t-\tau) = -M\left(d\gamma(\tau)/d\tau\right)$, with the convention that $\gamma(t) = 0$. Observe that besides the effects of noise and dissipation, the σ^2 term clearly acts to suppress the off-diagonal elements of the density matrix. Therefore we must add decoherence to the list of effects of the environment on the system, together with dissipation, diffusion and renormalization.

3.4 The Langevin equation

We now present two ways to derive the Langevin equation: first, formally from the influence action using the Feynman–Vernon identity [FeyVer63, FeyHib65]

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to reduce the part containing the noise kernel to an integral over a new classical stochastic forcing term, and second, through the time evolution of the reduced Wigner function. When the influence functional has the form (3.61), either rigorously or as a result of approximations, it is possible to read the Langevin equation directly off the path integral representation for the reduced density matrix, without explicit reference to the Wigner function. The idea is to substitute the Gaussian identity (3.76) into the path integral representation (3.51). We then commute the integrals, and perform the x and x' integrations by the method of stationary phase. The coupled equations for the stationary paths admit solutions where $x = x'$, and the Langevin equation (3.93) is just the stationarity condition for these solutions. The final integration over ξ is, of course, necessary to compute physical observables.

Later, in Chapter 5, when we treat open systems of quantum fields, we shall use this method as an efficient way to derive the functional Langevin equation. In Chapter 9 we will discuss in greater detail a class of problems where the fluctuations predicted by this Langevin equation have a direct physical meaning.

From the influence action via a noise average

For linear coupling to a linear bath, the influence functional has the form (3.61). In this case Feynman and Vernon showed that the noise kernel part of the influence functional can be written as a classical stochastic force ξ acting on the system. The following is an identity of the Gaussian functional integral:

$$\exp\left\{\frac{-1}{2\hbar}\int dtdt'\; u\left(t\right)\mathbf{N}\left(t,t'\right)u\left(t'\right)\right\} = \int D\xi\; P\left[\xi\right]\; \exp\left[\frac{i}{\hbar}\int_0^\infty dt\; \xi u\right] \tag{3.76}$$

where $P\left[\xi\right]$ is a Gaussian measure such that

$$\langle\xi\rangle = 0, \quad \langle\xi\left(t\right)\xi\left(t'\right)\rangle = \hbar\mathbf{N}\left(t,t'\right) \tag{3.77}$$

The stochastic force ξ has zero mean and correlation function given by $\mathbf{N}(t,t')$ the noise kernel, thus its name. We observe that $P\left[\xi\right]$ does not depend on t. The probability density functional is a functional of $X(s)$ if we allow the statistical properties of ξ to depend on the system history. This functional defines a stochastic average $\langle\;\rangle_\xi$ as a functional integral over $\xi(s)$ multiplied by a normalized Gaussian probability density functional $\mathcal{P}[\xi(s);X(s)]$.

One can then write the total influence functional (3.51) as

$$\mathcal{F}[X,u] = \left\langle \exp\left[\frac{i}{\hbar}\int_{t_i}^{t_f}\xi_{\text{full}}(s)u(s)ds\right]\right\rangle \tag{3.78}$$

$$\xi_{\text{full}}(s) = \int_{t_i}^{s} ds'\mathbf{D}(s,s')X(s') + \xi(s) \tag{3.79}$$

The equation of motion generated by the influence action is

$$\frac{\partial L}{\partial x} - \frac{d}{dt}\frac{\partial L}{\partial \dot{x}} + \int_{t_i}^{s} ds'\;\mathbf{D}(s,s')X(s') = -\xi(t) \tag{3.80}$$

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whereby we obtain the Langevin equation. In general $\mathbf{D}$ generates nonlocal dissipation while ξ represents a colored noise source.

The reduced Wigner function

We have seen that any wavefunction is associated with a function in phase space, the so-called Wigner function (cf. equation (3.15)). Suppose the system is described by a density matrix rather than a single wavefunction. Decomposing the density matrix in terms of its own eigenfunctions

$$\rho\left(x,x',t\right)=\sum_{\alpha}\rho_{\alpha}\left(t\right)\psi_{\alpha}\left(x,t\right)\psi_{\alpha}^{*}\left(x',t\right) \tag{3.81}$$

$$\int dx\ \psi_{\alpha}^{*}\left(x,t\right)\psi_{\beta}\left(x,t\right)=\delta_{\alpha\beta} \tag{3.82}$$

we see that $\rho_\alpha(t)$ is the probability of finding the system in one of the ψ_α states. Let us associate each ψ_α state with its corresponding Wigner function f_α^W, and compute the expectation value

$$\begin{aligned} f^{W}\left(x,p,t\right) &= \sum_{\alpha}\rho_{\alpha}\left(t\right)f_{\alpha}^{W}\left(x,p,t\right) \\ &= \int\frac{du}{2\pi\hbar}\,e^{-ipu/\hbar}\sum_{\alpha}\rho_{\alpha}\left(t\right)\ \psi_{\alpha}^{*}\left(x-\frac{u}{2},t\right)\psi_{\alpha}\left(x+\frac{u}{2},t\right) \\ &= \int\frac{du}{2\pi\hbar}\,e^{-ipu/\hbar}\,\rho\left(x+\frac{u}{2},x-\frac{u}{2},t\right) \end{aligned} \tag{3.83}$$

The Wigner function is directly given as the partial Fourier transform of the density matrix, without any explicit reference to the latter eigenstates.

For a quantum open system, we define the reduced Wigner function as the partial Fourier transform of the reduced density matrix

$$f_{r}^{W}\left(X,P,t\right)=\int\frac{du}{2\pi\hbar}\,e^{-iPu/\hbar}\,\rho_{r}\left(X+\frac{u}{2},X-\frac{u}{2},t\right) \tag{3.84}$$

From the path integral representation of the reduced density matrix containing its dynamics one can derive how the reduced Wigner function evolves in time [CaRoVe01, Rou02, CaRoVe03].

Let us replace ρ_r in equation (3.84) by its path integral representation, with the initial reduced density matrix given in terms of the initial reduced Wigner function

$$\begin{aligned} f_{r}^{W}\left(X_{f},P_{f},t\right) &= \int\frac{du_{f}}{2\pi\hbar}\,e^{-iP_{f}u_{f}/\hbar}\int_{x(t)=X_{f}+u_{f}/2,x'(t)=X_{f}-u_{f}/2}DxDx' \\ &\quad\times\exp\left\{\frac{i}{\hbar}\left[S_{S}\left[x\right]-S_{S}\left[x'\right]+S_{\mathrm{IF}}\left[x,x',t\right]\right]\right\} \\ &\quad\times\int dP_{i}\ \exp\left[\frac{i}{\hbar}P_{i}\left(x\left(0\right)-x'\left(0\right)\right)\right]\ f_{r}^{W}\left(\frac{x\left(0\right)+x'\left(0\right)}{2},P_{i},0\right) \end{aligned} \tag{3.85}$$

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Insert the momentum variables by means of the identity

$$e^{iS_S[x]/\hbar} = \exp\left[-\frac{i}{\hbar}\int_0^t dt\, V\left[x\left(t\right)\right]\right]\int Dp\, \exp\left\{\frac{i}{\hbar}\int_0^t dt\, \left[p\dot{x} - \frac{p^2}{2M}\right]\right\} \quad (3.86)$$

and introduce new variables

$$x, x' = X \pm \frac{u}{2} \quad (3.87)$$

$$p, p' = P \pm \frac{\pi}{2} \quad (3.88)$$

We assume a linear bath so the influence functional has the form (3.61). We then use the Gaussian identity (3.76) to introduce the stochastic variable ξ and write

$$V\left(x\right) - V\left(x'\right) = uV'\left(X\right) + \mathbf{V}\left(X, u\right), \qquad \mathbf{V} \sim O\left(u^3\right) \quad (3.89)$$

We may now formally integrate over the u and π variables, to get

$$\begin{aligned} f_r^W\left(X_f, P_f, t\right) = &\int_{X(t)=X_f, P(t)=P_f} DXDP\, f_r^W\left(X\left(0\right), P\left(0\right), 0\right) \\ &\times \int D\xi\, P_Q\left[\xi, t\right]\, \delta\left[\dot{P} + V'\left(X\right) + D\left(t\right) - \xi\right]\delta\left[\dot{X} - \frac{P}{M}\right] \end{aligned} \quad (3.90)$$

where

$$D\left(t\right) = -\int_0^t dt'\, \mathbf{D}\left(t, t'\right) X\left(t'\right) \quad (3.91)$$

$$P_Q\left[\xi, t\right] = \exp\left[\frac{-i}{\hbar}\int_0^t dt\, \mathbf{V}\left(X, i\hbar\frac{\delta}{\delta\xi\left(t\right)}\right)\right] P\left[\xi\right] \quad (3.92)$$

In other words, the Wigner function evolves as if it described an ensemble of particles following trajectories which obey the equations

$$\dot{X}\left(t\right) = \frac{P\left(t\right)}{M}, \qquad \dot{P}\left(t\right) = -V'\left(X\left(t\right)\right) - D\left(t\right) + \xi\left(t\right) \quad (3.93)$$

with random initial conditions weighted by the initial Wigner function and noise autocorrelation given by equation (3.77). These are the Hamilton equations of the system but now acquiring two extra terms, D and ξ, describing the influence of the environment. D is a deterministic, memory-dependent term, while ξ plays the role of "noise" with a "probability" distribution P_Q. Observe that this is an exact relation; in particular, the system retains fully its quantum coherence, which is encoded in P_Q. This means that we can use averages over the "noise" and initial conditions to compute exact quantum expectation values of system variables. In this sense, the Langevin equation gives the most detailed description of the quantum open system we shall see in this chapter.

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Incidentally, observe that since $\mathbf{V}$ involves cubic derivatives or higher, the noise autocorrelation is given by equation (3.77), independent of the self-interaction potential V.

The path integral representation (3.90) may be simplified greatly if the X dependence of $\mathbf{V}$ can be ignored (as it happens when the potential is cubic), or at least X may be replaced by the solution $\bar{X}\left[X\left(0\right), P\left(0\right), 0; t\right)$ to the classical equations of motion with Cauchy data $\left(X\left(0\right), P\left(0\right)\right)$ at time 0. In this case the path integral over X and P may be performed, and we get

$$f_r^W\left(X_f, P_f, t\right) = \left\langle \delta\left(X\left(t\right) - X_f\right)\delta\left(P\left(t\right) - P_f\right)\right\rangle \tag{3.94}$$

where $X(t)$ and $P\left(t\right)$ are the solutions of the Langevin equation (3.93) and the average is over the initial conditions and noise realizations. This average is more involved than the one we considered in Chapter 2, because of the more complex noise distribution function.

3.4.1 The linear bath model

It is interesting to compare equations (3.93) to the simple linear bath model we discussed in Chapter 2. To this end, we shall use expressions (3.62) for the dissipation and noise kernels. Let us write $q = \{q_\alpha\}$, $Q = \sum c_\alpha q_\alpha$. Recall that the expectation values in equation (3.62) are computed at $X = 0$, and that for a linear system the commutator of two field operators, being a c-number, is state independent. Thus, we may write

$$\left[Q\left(t\right), Q\left(t'\right)\right] = \sum c_\alpha^2\left[q_\alpha\left(t\right), q_\alpha\left(t'\right)\right] \tag{3.95}$$

For a linear system we may solve Heisenberg's equations

$$q_\alpha\left(t\right) = q_\alpha\left(0\right)\cos\omega_\alpha t + p_\alpha\left(0\right)\frac{\sin\omega_\alpha t}{m_\alpha\omega_\alpha} \tag{3.96}$$

$$\left[q_\alpha\left(t\right), q_\alpha\left(t'\right)\right] = \frac{\hbar}{i}\frac{\sin\omega_\alpha\left(t - t'\right)}{m_\alpha\omega_\alpha} \tag{3.97}$$

To compare with the Brownian motion model, we write

$$\mathbf{D}\left(t, t'\right) = -M\frac{\partial}{\partial t}\gamma\left(t - t'\right) \tag{3.98}$$

After an integration by parts, and discarding the term from the lower limit because we assume the interaction is switched on smoothly, we get

$$D\left(t\right) = M\delta\Omega_0^2 X\left(t\right) + \int_0^t dt'\,\gamma\left(t - t'\right)P\left(t'\right) \tag{3.99}$$

$$\gamma\left(t - t'\right) = \frac{1}{M}\sum_\alpha\frac{c_\alpha^2}{m_\alpha\omega_\alpha^2}\cos\omega_\alpha\left(t - t'\right)$$

$$\delta\Omega_0^2 = -\gamma\left(0\right)$$

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as in Chapter 2, equation (2.12). We now see the origin of the name *dissipation kernel* for $\mathbf{D}(t,t')$.

In reference to the noise, we observe first of all that

$$\frac{1}{2}\langle\{Q(t),Q(t')\}\rangle = \langle Q(t)\rangle\langle Q(t')\rangle + \frac{1}{2}\langle\{Q(t)-\langle Q(t)\rangle, Q(t')-\langle Q(t')\rangle\}\rangle \tag{3.100}$$

If, for example, the initial state for the environment is thermal, then $\langle Q(t)\rangle = 0$, and we recover the result from Chapter 2, equation (2.16)

$$\langle\xi(t)\xi(t')\rangle = \hbar\mathbf{N}(t,t') = \sum_\alpha \frac{c_\alpha^2}{m_\alpha\omega_\alpha^2}\langle\varepsilon_\alpha\rangle\cos\omega_\alpha(t-t') \tag{3.101}$$

only now we must use the quantum energy expectation value

$$\langle\varepsilon_\alpha\rangle = \hbar\omega_\alpha\left[\frac{1}{2}+\frac{1}{e^{\hbar\omega_\alpha/k_\mathrm{B}T}-1}\right] \tag{3.102}$$

whereby we recover the quantum form of the fluctuation–dissipation theorem. Of course, the noise is truly Gaussian only if $\mathbf{V}$ is zero, which means the system itself is linear.

If the bath frequencies span a continuum, we should replace

$$\sum_\alpha \to \int_0^\infty d\omega\,\rho(\omega) \tag{3.103}$$

where $\rho(\omega)\,d\omega$ is the number of oscillators with frequencies between ω and $\omega + d\omega$. We say the bath is ohmic if

$$\rho(\omega) = \frac{4\gamma M}{\pi}\frac{m_\omega\omega^2}{c(\omega)^2} \tag{3.104}$$

for some constant γ. Observe that for an ohmic bath $\gamma(t-t') = 4\gamma\delta(t-t')$ and $D(t) = 2\gamma P(t)$, so the Langevin equation is local in time. No physical bath can be exactly ohmic, because it would require either an infinite number of oscillators or else arbitrarily strong coupling to the bath, but many physical systems exhibit ohmic dissipation (for example, a biased Josephson junction) and may be modeled as *if* they were in contact with an ohmic bath.

Let us investigate the noise autocorrelation for an ohmic bath in equilibrium. We have

$$\langle\xi(t)\xi(t')\rangle = \hbar\mathbf{N}(t,t') = \frac{4\hbar M\gamma}{\pi}\int_0^\infty d\omega\,\omega\left[\frac{1}{2}+\frac{1}{e^{\hbar\omega/k_\mathrm{B}T}-1}\right]\cos\omega(t-t') \tag{3.105}$$

For high temperature and $t-t' \gg \hbar/k_\mathrm{B}T$, we may argue that the integral is dominated by low frequencies, whereby the noise is white and we recover the classical fluctuation–dissipation theorem

$$\hbar\mathbf{N}(t,t')|_{T\to\infty} = 4M\gamma k_\mathrm{B}T\delta(t-t') \tag{3.106}$$

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As $T \to 0$, however, the integral becomes singular. Let us define

$$\mathrm{Pf}\left[\frac{1}{t^2}\right] = -\int_0^\infty d\omega\ \omega \cos \omega t, \tag{3.107}$$

where Pf stands for the Hadamard finite part prescription. For example, if we regularize the integral by including a convergence factor $e^{-\omega/\Lambda}$, then

$$\mathrm{Pf}\left[\frac{1}{t^2}\right] = \lim_{\Lambda\to\infty} \frac{t^2 - \Lambda^{-2}}{\left(t^2 + \Lambda^{-2}\right)^2} \tag{3.108}$$

With this definition, the noise correlation at $T = 0$ becomes

$$\hbar \mathbf{N}\left(t, t'\right)|_{T=0} = -\frac{2\hbar M\gamma}{\pi}\ Pf\left[\frac{1}{\left(t - t'\right)^2}\right] \tag{3.109}$$

Observe that the decay of the noise correlation obeys a power law, which implies a very strongly colored noise.

3.5 The Kramers–Moyal equation

As in Chapter 2, the Langevin equation for the "trajectories" of the quantum open system may be turned into a Kramers–Moyal equation for the reduced Wigner function. To obtain this equation, we simply take the time derivative of the path integral representation (3.90). Observe that we get a new term coming from the explicit time dependence of P_Q. Indeed, write

$$P_Q\left[\xi, t\right] = P_Q\left[\xi, t^*\right] - \frac{i}{\hbar}\left(t - t^*\right)\ \mathbf{V}\left(X_f, i\hbar\frac{\delta}{\delta\xi\left(t^*\right)}\right) P_Q\left[\xi, t^*\right] \tag{3.110}$$

where the reference time $t^* < t$ is taken to t after computing the derivatives. Then the noise averages may be split in two, and

$$\frac{\partial}{\partial t} f_r^W\left(X_f, P_f, t\right) = -\left\{H, f_r^W\right\} + M\delta\Omega_0^2 X_f \frac{\partial f_r^W}{\partial P_f} + \frac{\partial}{\partial P_f}\left[\mathbf{A} + \mathbf{B}\right] + \mathbf{C} \tag{3.111}$$

where the first term contains the Poisson brackets. The new terms are

$$\mathbf{A} = \int_0^t dt'\ \gamma\left(t - t'\right)\left\langle P\left(t'\right)\ \delta\left(X\left(t\right) - X_f\right)\delta\left(P\left(t\right) - P_f\right)\right\rangle \tag{3.112}$$

$$\mathbf{B} = -\left\langle \xi\left(t\right)\ \delta\left(X\left(t\right) - X_f\right)\delta\left(P\left(t\right) - P_f\right)\right\rangle \tag{3.113}$$

$$\mathbf{C} = \left(\frac{-i}{\hbar}\right)\left\langle \mathbf{V}\left(X_f, -i\hbar\frac{\delta}{\delta\xi\left(t^*\right)}\right)\ \delta\left(X\left(t\right) - X_f\right)\delta\left(P\left(t\right) - P_f\right)\right\rangle \tag{3.114}$$

We may use certain approximations to extract the leading behavior of these expressions. To simplify the $\mathbf{A}$ term, for example, we replace $P\left(t'\right)$ by the solution $\bar{P}\left[X_f, P_f, t; t'\right)$ to the classical equations of motion with Cauchy data $\left[X_f, P_f\right]$ at time t. Observe that even for a strong system–bath interaction this

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approximation is justified if the kernel γ decays fast enough; it is exact for an ohmic bath. So we approximate

$$\mathbf{A} \sim \mathbf{\Gamma}\left(X_f, P_f, t\right) f_r^W\left(X_f, P_f, t\right) \tag{3.115}$$

$$\mathbf{\Gamma}\left(X_f, P_f, t\right) = \int_0^t dt'\, \gamma\left(t-t'\right) \bar{P}\left[X_f, P_f, t; t'\right) \tag{3.116}$$

To simplify the $\mathbf{B}$ term, let us first neglect the X dependence in $\mathbf{V}$. This approximation is actually exact for a cubic potential. Also recall that since the t dependence of $\mathbf{V}$ is explicitly considered through the $\mathbf{C}$ term, the time-integral in P_Q in the $\mathbf{B}$ term is truncated at t^-. Then we have

$$\begin{aligned} -\xi\left(t\right) P_Q\left[\xi, t\right] &= -\exp\left[\frac{-i}{\hbar}\int_0^{t^-} dt'\, \mathbf{V}\left(X, i\hbar\frac{\delta}{\delta\xi\left(t\right)}\right)\right] \xi\left(t\right) P\left[\xi\right] \\ &= \int_0^t dt'\, \hbar\mathbf{N}\left(t-t'\right) \frac{\delta}{\delta\xi\left(t'\right)} P_Q\left[\xi, t\right] \end{aligned} \tag{3.117}$$

and after a further integration by parts

$$\begin{aligned} \mathbf{B} = \int_0^t dt'\, \hbar\mathbf{N}\left(t-t'\right) \Bigg\{ &\left\langle \frac{\delta X\left(t\right)}{\delta\xi\left(t'\right)} \frac{\partial}{\partial X_f} \delta\left(X\left(t\right) - X_f\right) \delta\left(P\left(t\right) - P_f\right) \right\rangle \\ &+ \left\langle \frac{\delta P\left(t\right)}{\delta\xi\left(t'\right)} \delta\left(X\left(t\right) - X_f\right) \frac{\partial}{\partial P_f} \delta\left(P\left(t\right) - P_f\right) \right\rangle \Bigg\} \end{aligned} \tag{3.118}$$

To compute the variations with respect to the noise, recall the identities

$$\frac{\delta X\left(t'\right)}{\delta\xi\left(t'\right)} = 0; \qquad \frac{\delta P\left(t'^+\right)}{\delta\xi\left(t'\right)} = 1 \tag{3.119}$$

and use the chain rule

$$0 = \frac{\delta X\left(t'\right)}{\delta X\left(t\right)} \frac{\delta X\left(t\right)}{\delta\xi\left(t'\right)} + \frac{\delta X\left(t'\right)}{\delta P\left(t\right)} \frac{\delta P\left(t\right)}{\delta\xi\left(t'\right)} \tag{3.120}$$

$$1 = \frac{\delta P\left(t'\right)}{\delta X\left(t\right)} \frac{\delta X\left(t\right)}{\delta\xi\left(t'\right)} + \frac{\delta P\left(t'\right)}{\delta P\left(t\right)} \frac{\delta P\left(t\right)}{\delta\xi\left(t'\right)} \tag{3.121}$$

Now assume that $\left(X, P\right)\left(t\right)$ and $\left(X, P\right)\left(t'\right)$ are linked through the classical equations of motion. The determinant of the system is 1 from Liouville's theorem, and so

$$\frac{\delta X\left(t\right)}{\delta\xi\left(t'\right)} = -\frac{\delta\bar{X}\left[X_f, P_f, t; t'\right)}{\delta P_f}; \qquad \frac{\delta P\left(t\right)}{\delta\xi\left(t'\right)} = \frac{\delta\bar{X}\left[X_f, P_f, t; t'\right)}{\delta X_f} \tag{3.122}$$

The final result is

$$\mathbf{B} = -\left\{\Phi, f_r^W\right\}, \tag{3.123}$$

$$\Phi = \int_0^t dt'\, \hbar\mathbf{N}\left(t-t'\right) \bar{X}\left[X_f, P_f, t; t'\right) \tag{3.124}$$

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Finally, to compute $\mathbf{C}$ we use the identities (3.119) at time t to get

$$\mathbf{C} = \left(\frac{-i}{\hbar}\right) \mathbf{V}\left(X_f, i\hbar\frac{\delta}{\delta P_f}\right) f_r^W\left(X_f, P_f, t\right) \tag{3.125}$$

To summarize, the quantum Kramers–Moyal equation reads

$$\begin{aligned}
&\frac{\partial}{\partial t} f_r^W\left(X_f, P_f, t\right) \\
&\quad = -\left\{H, f_r^W\right\} - \left(\frac{i}{\hbar}\right) \mathbf{V}\left(X_f, i\hbar\frac{\delta}{\delta P_f}\right) f_r^W\left(X_f, P_f, t\right) \\
&\qquad + M\delta\Omega_0^2 X_f \frac{\partial f_r^W}{\partial P_f} \\
&\qquad + \frac{\partial}{\partial P_f}\left[\mathbf{\Gamma}\left(X_f, P_f, t\right) f_r^W\left(X_f, P_f, t\right) - \left\{\Phi, f_r^W\right\}\right]
\end{aligned} \tag{3.126}$$

The first line gives the evolution of the Wigner function without interaction with the environment, while the second and third lines describe the renormalization, dissipation, diffusion and decoherence effects.

3.5.1 The linear system model

If the system itself is linear, we can obtain simple analytic expressions for $\bar{X}\left[X_f, P_f, t; t'\right)$ and $\bar{P}\left[X_f, P_f, t; t'\right)$ and thus derive an explicit result. We have (cf. equation (3.70))

$$\bar{X}\left[X_f, P_f, t; t'\right) = X_f \cos\Omega\left(t - t'\right) - \frac{P_f}{M\Omega}\sin\Omega\left(t - t'\right) \tag{3.127}$$

$$\bar{P}\left[X_f, P_f, t; t'\right) = P_f \cos\Omega\left(t - t'\right) + M\Omega X_f \sin\Omega\left(t - t'\right) \tag{3.128}$$

The Kramers–Moyal equation now reads (for a linear system, $\mathbf{V} = 0$)

$$\begin{aligned}
\frac{\partial}{\partial t} f_r^W\left(X_f, P_f, t\right) = &-\left\{H, f_r^W\right\} + M\delta\Omega^2\left(t\right) X_f \frac{\partial f_r^W}{\partial P_f} \\
&+ \frac{\partial}{\partial P_f}\left[2\Gamma\left(t\right) P_f + \frac{\sigma^2\left(t\right)}{2}\frac{\partial}{\partial P_f} + \Delta_{ad}\left(t\right)\frac{\partial}{\partial X_f}\right] f_r^W
\end{aligned} \tag{3.129}$$

where the coefficients $\sigma^2\left(t\right)$, $\Delta\left(t\right)$, $\Gamma\left(t\right)$ and $\delta\Omega^2\left(t\right)$ were defined above, from equations (3.72)–(3.75). The identity of the coefficients to those in the master equation (3.71) is not surprising, since for linear systems the Kramers–Moyal equation (3.129) and the master equation (3.71) are equivalent. For nonlinear systems, they are still closely related, but the approximations which go into one or the other are not exactly the same.

The form (3.129) of the Kramers–Moyal equation makes it clear that the coefficient $\gamma\left(t\right)$ is associated with dissipation and $\sigma^2\left(t\right)$ with "normal" diffusion. We call $\Delta_{ad}\left(t\right)$ the "anomalous" diffusion constant.

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$\sigma^2(t)$ also pertains to decoherence. To see this, consider the pseudo-entropy

$$\begin{aligned}\tilde{S} &= 1 - \mathrm{tr}\,\rho_r^2 \\ &= 1 - (2\pi\hbar)\int dX dP\,(f_r^W)^2(X,P)\end{aligned} \tag{3.130}$$

Then

$$\frac{d\tilde{S}}{dt} = 2\Gamma(1-\tilde{S}) + (4\pi\hbar)\int dX dP\left\{\frac{\sigma^2(t)}{2}\left(\frac{\partial f_r^W}{\partial P_f}\right)^2 + \Delta_{ad}(t)\frac{\partial f_r^W}{\partial X_f}\frac{\partial f_r^W}{\partial P_f}\right\} \tag{3.131}$$

The first term represents heat loss to the environment and the second induces decoherence. The third does not have a definite sign.

To conclude, let us evaluate these coefficients for an ohmic bath. At high temperature, we get the expected relations $\Gamma(t) = \gamma$, $\sigma^2(t) = 4\gamma M k_{\mathrm{B}} T$, $\Delta_{ad}(t) = \delta\Omega^2(t) = 0$. At $T = 0$, though, the naive expressions diverge. Suppose we use an exponential cut-off to regularize them, as in (3.108). Then as the cut-off is removed, we get $\Gamma(t) = \gamma$ and $\delta\Omega^2(t) = 0$. For the expressions involving the noise kernel (3.109), we get that Δ_{ad} diverges logarithmically, while σ^2 diverges linearly in the cut-off Λ. This result suggests that at late times the system perceives the environment as a heat bath at a temperature $k_{\mathrm{B}}T_{\mathrm{eff}} \approx \hbar\Lambda$ [ALMV06].

3.6 Derivation of the propagator and the master equation

For the influence functional path integral treatment of quantum Brownian motion (QBM) the formal expression of the evolutionary operator for the reduced density matrix was derived by Grabert, Schramm and Ingold [GrScIn88] and an exact master equation for QBM in a general (non-ohmic) environment at an arbitrary temperature was derived by Hu, Paz and Zhang [HuPaZh92, HuPaZh93a]. In this section we give a discussion of this problem based on their work. This is useful not only as a model example of this important method, but also because in some problems such as the calculation of entropy generation (to be discussed in Chapter 9) in quantum open systems we need some of these details.

Let us consider the general case of a quantum harmonic oscillator with time-dependent mass, cross-term and natural frequency undergoing Brownian motion through its interaction with an environment made up of n harmonic oscillators with the same time-dependent parameters. The total Lagrangian of the system is given by

$$\begin{aligned}S[x,\mathbf{q}] &= S[x] + S_E[\mathbf{q}] + S_{\mathrm{int}}[x,\mathbf{q}] \\ &= \int_{t_i}^{t} ds\Bigg\{\frac{1}{2}M(s)\left[\dot{x}^2 + 2\mathcal{E}(s)x\dot{x} - \Omega^2(s)x^2\right] \\ &\quad + \sum_n\left[\frac{1}{2}m_n(s)\left[\dot{q}_n^2 + 2\varepsilon_n(s)q_n\dot{q}_n - \omega_n^2(s)q_n^2\right]\right] + \sum_n\left[-c(s)xq_n\right]\Bigg\}\end{aligned} \tag{3.133}$$

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where the particle and the bath oscillators have coordinates x and q_n, respectively; we may also let the system variable interact with the environment variable through a more general $f(x)$ functional form. This Hamiltonian is considered in detail by Hu and Matacz [HuMat94] as an example of a squeezed quantum open system. We will discuss this in the last section of Chapter 4.

3.6.1 Evolution of the reduced density matrix

Given some initial system density matrix $\rho_S(x_i\, x_i'\, 0)$ we want to evolve it in time using (3.49). The formal expression for $\mathcal{J}_r$ was derived by Grabert *et al.* [GrScIn88] using path integral methods, and calculated explicitly in [HuPaZh92, HuPaZh93a, HuMat94] for a general (non-ohmic) environment.

In terms of the sum and difference variables the classical paths followed by the system, $X_{\rm cl}, u_{\rm cl}$, can be written in terms of more elementary functions u, v:

$$\begin{aligned} X_{\rm cl}(s) &= X_{\rm cl}(t_i)u_1(s) + X_{\rm cl}(t)u_2(s) \\ u_{\rm cl}(s) &= u_{\rm cl}(t_i)v_1(s) + u_{\rm cl}(t)v_2(s) \end{aligned} \tag{3.134}$$

Then it can be shown [HuMat94] that the evolutionary operator $\mathcal{J}_r$ is equal to

$$\begin{aligned} \mathcal{J}_r(x, x', t|x_i, x_i', t_i) = \frac{|b_2|}{2\pi\hbar} \exp\Bigg[&\frac{i}{\hbar}(b_1 X u - b_2 X u_i + b_3 X_i u - b_4 X_i u_i) \\ &- \frac{1}{\hbar}\left(a_{11}u_i^2 + a_{12}u_i u + a_{22}u^2\right)\Bigg] \end{aligned} \tag{3.135}$$

The functions $b_1 \to b_4$ can be expressed as

$$\begin{aligned} b_1(t, t_i) &= M(t)\dot{u}_2(t) + M(t)\mathcal{E}(t) \\ b_2(t, t_i) &= M(t_i)\dot{u}_2(t_i) \\ b_3(t, t_i) &= M(t)\dot{u}_1(t) \\ b_4(t, t_i) &= M(t_i)\dot{u}_1(t_i) + M(t_i)\mathcal{E}(t_i) \end{aligned} \tag{3.136}$$

while the functions a_{ij} are defined by

$$a_{ij}(t, t_i) = \frac{1}{1+\delta_{ij}} \int_{t_i}^{t} ds \int_{t_i}^{t} ds'\; v_i(s)\; \mathbf{N}(s, s')\; v_j(s') \tag{3.137}$$

The functions $u_1 \to v_2$ are solutions to the following equations (dropping subscripts on u, v):[1]

$$\ddot{u}(s) + \frac{\dot{M}}{M}\dot{u} + \left(\Omega^2 + \dot{\mathcal{E}} + \frac{\dot{M}}{M}\mathcal{E}\right) u - \frac{1}{M(s)} \int_{t_i}^{s} ds'\; \mathbf{D}(s, s')\; u(s') = 0 \tag{3.138}$$

$$\ddot{v}(s) + \frac{\dot{M}}{M}\dot{v} + \left(\Omega^2 + \dot{\mathcal{E}} + \frac{\dot{M}}{M}\mathcal{E}\right) v - \frac{1}{M(s)} \int_{s}^{t} ds'\; v(s')\mathbf{D}(s', s) = 0 \tag{3.139}$$

[1] Do not confuse u here with $\mathbf{u} \equiv \mathbf{x}_1 - \mathbf{x}_2$ in Chapter 2 or $u \equiv x - x'$ in Chapter 3.

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subject to the boundary conditions

$$u_1(t_i) = v_1(t_i) = 1, \quad u_1(t) = v_1(t) = 0 \tag{3.140}$$

$$u_2(t_i) = v_2(t_i) = 0, \quad u_2(t) = v_2(t) = 1 \tag{3.141}$$

To proceed further we need explicit expressions for $a_{11} \to b_4$. These are expressed in terms of $u_1 \to v_2$, which in turn come from solving equations (3.138) and (3.139). To solve these equations we need to know the dissipation $\mathbf{D}$ kernel of the environment, which is determined by the coupling and the spectral density function of the environment. We consider an ohmic bath and assume an unsqueezed (coherent) thermal bath made up of unit mass static (time-independent frequency) oscillators so the dissipation and noise kernels simplify to the form

$$\begin{aligned} \mathbf{D}(s,s') &= -4\gamma_0\, c(s)c(s')\,\delta'(s-s') \\ \mathbf{N}(s,s') &= \frac{2\gamma_0}{\pi}\, c(s)c(s') \int_0^\infty \omega \coth \frac{\hbar\omega}{2k_{\mathrm{B}}T} \cos\omega(s-s')\, d\omega \end{aligned} \tag{3.142}$$

If $c(s) = c =$ constant, we may identify $\gamma_0 c^2 = M\gamma$. In this case, in the high-temperature limit the noise becomes white, that is, $\mathbf{N}$ tends toward a delta function.

3.6.2 Master equation

We now proceed with the derivation of the master equation from the evolution operator using the simplified method of Paz [Paz94]. We first take the time derivative of both sides of equation (3.135), multiply both sides by $\rho_r(X_i, u_i, t_i)$ and integrate over X_i, u_i to obtain

$$\begin{aligned} \dot\rho_r(X_f,u_f,t) = &\left[\frac{\dot b_2}{b_2} + \frac{i}{\hbar}\dot b_1 X_f u_f - \dot a_{22}\frac{u_f^2}{\hbar}\right]\rho_r(X_f,u_f,t) \\ &+ \frac{i}{\hbar}u_f \dot b_3 \int du_i dX_i\, X_i \mathcal{J}_r \rho_r(X_i,u_i,t_i) \\ &- \frac{1}{\hbar}(i\dot b_2 X_f + \dot a_{12} u_f)\int du_i dX_i\, u_i \mathcal{J}_r \rho_r(X_i,u_i,t_i) \\ &- \frac{i}{\hbar}\dot b_4 \int du_i dX_i\, X_i u_i \mathcal{J}_r \rho_r(X_i,u_i,t_i) \\ &- \frac{\dot a_{11}}{\hbar}\int du_i dX_i\, u_i^2 \mathcal{J}_r \rho_r(X_i,u_i,t_i) \end{aligned} \tag{3.143}$$

Here the dot denotes the derivative with respect to t. We can perform the

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integrals in (3.143) by using

$$u_i \mathcal{J}_r = \frac{i\hbar}{b_2}\frac{\partial \mathcal{J}_r}{\partial X_f} + \frac{b_1 u_f}{b_2}\mathcal{J}_r \tag{3.144}$$

$$X_i \mathcal{J}_r = -\frac{i}{b_3}\left[\hbar\frac{\partial \mathcal{J}_r}{\partial u_f} + (u_i a_{12} + 2u_f a_{22})\mathcal{J}_r)\right] - \frac{b_1}{b_3}X_f \mathcal{J}_r \tag{3.145}$$

$$\begin{aligned} X_i u_i \mathcal{J}_r = &-\left(\frac{i\hbar}{b_2}\frac{\partial}{\partial X_f} + \frac{b_1 u_f}{b_2}\right) \\ &\times\left(\frac{i\hbar}{b_3}\frac{\partial}{\partial u_f} + \frac{i}{b_3}[u_i a_{12} + 2u_f a_{22}] + \frac{b_1}{b_3}X_f\right)\mathcal{J}_r \end{aligned} \tag{3.146}$$

The u_i functions obey mixed boundary conditions. It is convenient to express them in terms of functions w_i obeying initial conditions only. We write

$$u_1(s) = w_1(s) - w_2(s)\frac{w_1(t)}{w_2(t)}, \quad u_2(s) = \frac{w_2(s)}{w_2(t)} \tag{3.147}$$

In order to satisfy the boundary conditions (3.140) we require

$$w_1(t_i) = \dot{w}_2(t_i) = 1, \quad w_2(t_i) = \dot{w}_1(t_i) = 0 \tag{3.148}$$

In this representation we can show that

$$\frac{\dot{b}_4}{b_2 b_3} = -\frac{1}{M(t)}, \quad b_1 = -M(t)\frac{\dot{b}_2}{b_2} + M(t)\mathcal{E}, \quad \dot{a}_{11} = -\dot{v}_1(t)a_{12} \tag{3.149}$$

With these relations the master equation is the same as equation (3.71) with two additional terms

$$\begin{aligned} i\hbar\frac{\partial}{\partial t}\,\rho_r(x,x',t) = &\left\{-\frac{\hbar^2}{2M(t)}\left(\frac{\partial^2}{\partial x^2} - \frac{\partial^2}{\partial x'^2}\right) + i\hbar\mathcal{E}\left(x\frac{\partial}{\partial x} + x'\frac{\partial}{\partial x'}\right)\right. \\ &\left. + \frac{M(t)}{2}\left[\Omega^2 + \delta\Omega^2(t)\right]\left(x^2 - x'^2\right) + i\hbar\mathcal{E}\right\}\rho_r(x,x',t) \\ &- i\hbar\Gamma(t,t_i)(x-x')\left(\frac{\partial}{\partial x} - \frac{\partial}{\partial x'}\right)\rho_r(x,x',t) \\ &- i\frac{\sigma^2(t)}{2\hbar}(x-x')^2\,\rho_r(x,x',t) \\ &+ \Delta_{ad}(t)(x-x')\left(\frac{\partial}{\partial x} + \frac{\partial}{\partial x'}\right)\rho_r(x,x',t) \\ &- i\hbar^2 D_{xx}(t,t_i)\left(\frac{\partial}{\partial x} + \frac{\partial}{\partial x'}\right)^2\rho_r(x,x',t) \end{aligned} \tag{3.150}$$

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where we identify

$$\left[\Omega^2 + \delta\Omega^2(t)\right] = \frac{b_1\dot{b}_3}{M(t)b_3} - \frac{\dot{b}_1}{M(t)} + \mathcal{E}^2 - \frac{\dot{b}_2}{b_2}\mathcal{E} \tag{3.151}$$

$$\Gamma(t,t_i) = -\frac{1}{2}\left(\frac{\dot{b}_3}{b_3} - \frac{\dot{b}_2}{b_2}\right) \tag{3.152}$$

$$-\frac{\sigma^2(t)}{2\hbar} = \frac{b_1^2}{b_2}\left(\frac{a_{12}}{M(t)} - \frac{\dot{a}_{11}}{b_2}\right) + \frac{2b_1}{M(t)}a_{22} - \dot{a}_{22} + 2\frac{\dot{b}_3}{b_3}a_{22} + a_{12}\frac{b_1\dot{b}_3}{b_2b_3} - \dot{a}_{12}\frac{b_1}{b_2} \tag{3.153}$$

$$\Delta_{ad}(t) = \hbar\left[\frac{\dot{a}_{12}}{b_2} - 2\frac{a_{22}}{M(t)} - \frac{\dot{b}_3a_{12}}{b_3b_2} - \frac{2b_1}{b_2}\left(\frac{a_{12}}{M(t)} - \frac{\dot{a}_{11}}{b_2}\right)\right] \tag{3.154}$$

$$D_{xx}(t,t_i) = \frac{1}{b_2}\left(\frac{a_{12}}{M(t)} - \frac{\dot{a}_{11}}{b_2}\right) \tag{3.155}$$

The dot in these equations denotes taking the derivative with respect to t.

The factor $a_{12}/M(t) - \dot{a}_{11}/b_2$ vanishes only when the dissipation kernel is stationary (i.e. a function of $s - s'$) and the system is a time-independent harmonic oscillator. When this happens $v_1(s) = u_2(t-s)$ and we have $\dot{v}_1(t) = -b_2/M(t)$. We see from equation (3.149) that the factor $a_{12}/M(t) - \dot{a}_{11}/b_2$ is zero in this case. All the diffusion coefficients contain this factor and D_{xx} depends solely on it.

3.7 Consistent histories and decoherence functional

The question which remains unanswered is whether individual solutions of the Langevin equation are actually observable. This question contains two aspects, namely, (a) whether the evolution of the quantum open system may be analyzed in terms of trajectories, and (b) whether these trajectories describe any recognizable dynamics. As we shall see, the answer is not straightforward, because it involves a new component, namely, the accuracy of our observations. Out of quantum common sense, we expect that if we follow the trajectories too closely, we would be feeding noise into the system (Heisenberg's principle), eventually masking the system–environment interaction. Still the question remains whether there is *any* range where the Langevin equation is a satisfactory description of the observed evolution of the system.

To analyze this question we shall adopt the consistent histories approach to quantum mechanics, in the version advanced by Gell-Mann and Hartle (see [Gri84, Gri93, Omn88, Omn90, Omn92, KoEzMuNo90, Har92, Har93, GelHar90, HarGel93, Bru93, GelHar06]). The idea is to define a history by a set of projectors P_α acting at times t_i. In canonical terms, a history is given by an evolution of the state vector such that at every time t_i, it belongs to the proper space of

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$P_\alpha(t_i)$. In path integral terms, the projectors are represented by window functions $w_\alpha[x(t_i)]$, which take on unit value if the instantaneous configuration x satisfies the requirements of the history α, and vanish otherwise. The limiting case of a *fine-grained history*, namely, when $x(t)$ is specified for all times, is assigned an amplitude $\exp iS/\hbar$, as usual in the Feynman path integral formulation. The amplitude for a *coarse-grained* history defined by window functions $w_\alpha[x(t_i)]$ is defined by the superposition

$$A[\alpha] = \int Dx\, e^{iS/\hbar}\psi[x(0)]\left\{\prod_i w_\alpha[x(t_i)]\right\} \tag{3.156}$$

The probability is naturally expressed in terms of a closed time path integral

$$\mathbf{P}[\alpha] = |A[\alpha]|^2 = \int DxDx'\, e^{i[S-S']/\hbar}\rho[x(0), x'(0)] \times\left\{\prod_i w_\alpha[x(t_i)]\right\}\left\{\prod_i w_\alpha[x'(t_i)]\right\} \tag{3.157}$$

In this way we may assign a probability to any coarse-grained history, but these probability assignments are not generally *consistent*, namely, the probabilities of two mutually exclusive histories do not generally add up. Indeed, let us define the *decoherence functional* of two histories α and β

$$\mathcal{D}[\alpha,\beta] = \int DxDx'\, e^{i[S-S']/\hbar}\rho[x(0), x'(0)]\left\{\prod_i w_\alpha[x(t_i)]\right\}\left\{\prod_j w_\beta[x'(t_j)]\right\} \tag{3.158}$$

$\mathbf{P}[\alpha] = \mathcal{D}[\alpha,\alpha]$ but $\mathbf{P}[\alpha\vee\beta] = \mathcal{D}[\alpha,\alpha] + \mathcal{D}[\beta,\beta] + 2\mathrm{Re}\mathcal{D}[\alpha,\beta] \neq \mathbf{P}[\alpha] + \mathbf{P}[\beta]$. The probability sum rule $\mathbf{P}[\alpha\vee\beta] = \mathbf{P}[\alpha] + \mathbf{P}[\beta]$ only applies when the third term vanishes, and in particular when there is *strong decoherence*, $\mathcal{D}[\alpha,\beta] = 0$ for $\alpha \neq \beta$. As physicists, who deal with reality, we shall be satisfied that a set of mutually exclusive histories is consistent when $|\mathcal{D}[\alpha,\beta]| \ll \mathcal{D}[\alpha,\alpha], \mathcal{D}[\beta,\beta]$ whenever $\alpha \neq \beta$.

A simple set of consistent histories refers to the values of conserved quantities [HaLaMa95]. First observe that the path integral expression (3.158) translates into the canonical expression

$$\mathcal{D}[\alpha,\beta] = \mathrm{Tr}\left\{\tilde{T}\left[\prod_j P_\beta(t_j)\right] T\left[\prod_i P_\alpha(t_i)\right]\rho(0)\right\} \tag{3.159}$$

The projectors at different times are related in the usual way $P_\alpha(t) = U(t)P_\alpha(0)U^\dagger(t)$. If a projector commutes with the Hamiltonian, then it is time-independent, and expression (3.159) collapses unless all projectors are indeed identical. The only histories with nonzero probabilities are those defined by ranges of conserved quantities in the initial state, and they are automatically consistent if these ranges do not overlap.

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For open quantum systems we are interested in histories where the system variable X is specified to follow a trajectory $\chi(t)$ with a given accuracy $\sigma(t)$, while the environment variable q is left unspecified. For technical reasons, it is convenient to use Gaussian, rather than sharp, windows. We also make a Gaussian ansatz for the initial state, which we assume to be pure. Therefore, we replace

$$\rho\left[x(0), x'(0)\right]\left\{\prod_i w_\alpha\left[x(t_i)\right]\right\}\left\{\prod_j w_\beta\left[x'(t_j)\right]\right\} \tag{3.160}$$

by

$$\exp\left[-\int \frac{dt}{2\sigma^2(t)}\left\{(x-\chi)^2+(x'-\chi')^2\right\}\right] \tag{3.161}$$

The unconstrained integration over environment variables yields the action functional, which has the structure we already know. Adopting a shorthand notation

$$\begin{aligned}\mathcal{D}[\chi,\chi'] = \int DxDx' \ \exp\left(\frac{-1}{2}\right) \\ \times\left\{-2iuLX+\mathbf{N}u^2+\frac{1}{\sigma^2}\left[(x-\chi)^2+(x'-\chi')^2\right]\right\}\end{aligned} \tag{3.162}$$

where $X = x + x'/2$, $u = x - x'$, the symbols L, $\mathbf{N}$ and $1/\sigma^2$ denote operators (which we shall handle as if they were c-numbers) and we have applied Einstein's convention to time integrals. Write $\chi, \chi' = \Upsilon \pm y/2$ and develop the last term to get

$$\begin{aligned}\mathcal{D}[\chi,\chi'] = \exp\left(\frac{-1}{2\sigma^2}\right)\left[2\Upsilon^2+\frac{y^2}{2}\right] \\ \times\int DXDu \ \exp\left(\frac{-1}{2}\right)\left\{-2iuLX+\left[\mathbf{N}+\frac{1}{2\sigma^2}\right]u^2+\frac{2}{\sigma^2}X^2\right\} \\ \times\exp\frac{1}{2\sigma^2}\left[uy+4X\Upsilon\right]\end{aligned} \tag{3.163}$$

Now consider the matrix

$$M = \begin{pmatrix} 2\sigma^{-2} & (-i)L \\ (-i)L & \mathbf{N}+\left(2\sigma^2\right)^{-1}\end{pmatrix} \tag{3.164}$$

Already from the fact that the noise kernel appears in the combination $\mathbf{N} + \left(2\sigma^2\right)^{-1}$ we see that there must be a limit where the "Langevin noise" is drowned in the "Heisenberg noise." The determinant of this matrix is $\mathrm{Det}(M) = \left(\mathbf{N}+\left(2\sigma^2\right)^{-1}\right)2\sigma^{-2}+L^2$, and the inverse is (we assume all operators commute)

$$M^{-1} = \left[\mathrm{Det}(M)\right]^{-1}\begin{pmatrix}\mathbf{N}+\left(2\sigma^2\right)^{-1} & iL \\ iL & 2\sigma^{-2}\end{pmatrix} \tag{3.165}$$

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Therefore

$$|\mathcal{D}[\chi,\chi']| \sim \exp\left\{-\left[\mathbf{1}-\frac{2\,[Det\,(M)]^{-1}}{\sigma^2}\left(\mathbf{N}+\left(2\sigma^2\right)^{-1}\right)\right]\frac{\Upsilon^2}{\sigma^2}\right.$$
$$\left.-\left[\mathbf{1}-\frac{[Det\,(M)]^{-1}}{\sigma^4}\right]\frac{y^2}{4\sigma^2}\right\} \tag{3.166}$$

We see that the dynamics and the decoherence aspects are clearly separated. To obtain a simpler expression, we shall assume that the L operator is "small," so we can expand in powers of L. Keeping only the first nonzero contributions, we get

$$|\mathcal{D}[\chi,\chi']| \sim \exp\left(\frac{-1}{2}\right)\left\{\left(\mathbf{N}+\left(2\sigma^2\right)^{-1}\right)^{-1}(L\Upsilon)^2+\mathbf{N}\left(2\sigma^2\mathbf{N}+1\right)^{-1}y^2\right\} \tag{3.167}$$

To find the probability of a given history, we must set $y=0$. We see that the most likely histories are those which satisfy the "classical" equations of motion $L\chi=0$; these are the equations of motion for the expectation value of the system variable, and include the dissipative terms, but not the noise. The magnitude of the expected deviations from the deterministic behavior is given by $\mathbf{N}+\left(2\sigma^2\right)^{-1}$. The noise kernel provides a lower bound for the "noisiness" of the dynamics, but we can say that the deviations from the classical motion are well described by the Langevin equation only in the limit of "fuzzy" observations, $\left(2\sigma^2\right)^{-1}\ll\mathbf{N}$. In the opposite limit, the dominant effect is the Heisenberg noise.

To study consistency, we must follow the decoherence functional as y increases. We see that our histories tend to decohere, and they become approximately consistent whenever $y^2\geq\left(2\sigma^2+\mathbf{N}^{-1}\right)$. The relevant question is whether any two histories which may be resolved by our apparatus are automatically consistent. The limit of resolution is $y^2\sim\sigma^2$; therefore, consistency is obtained only asymptotically for strong noise $\sigma^2\mathbf{N}\gg 1$.

In conclusion, a picture of the system evolution based on actual nearly classical trajectories may only result from a compromise whereby the accuracy of observations is adjusted to the noise level, $\sigma^2\sim\mathbf{N}^{-1}$. Larger noise for a given σ means more decoherence but less predictability; for a weaker noise, predictability is only limited by the Heisenberg bounds, but individual trajectories will not decohere. If we are satisfied with predictability within the limits imposed by the Langevin equation, then in the strong noise limit we may consider individual trajectories as actually depicting physical reality.

For a critique of the consistent history approach to quantum mechanics, see [DowKen96, BasGhi99].

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