

## Week 7

PHY 435 / 635 Decoherence and Open Quantum Systems

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In the remaining parts of section 4 on "Markovian OQS", we apply the Master equation concept to most of the system-environment models introduced in section 2.

### 4.4 Quantum Brownian Motion

**Classical Brownian Motion:** First checkout the [classical version](#) . See this [video](#) .

We begin with a central harmonic oscillator coupled to an environment of oscillators, please revise the complete Hamiltonian  $\hat{H}$  and setup in section 2.1. Our objective is to derive the Born-Markov Master equation (4.21), following from  $\hat{H}$ .

Returning to the system-environment coupling term (2.3) we see that we had written it as

$$\hat{H}_{\text{int}} = \hat{X} \otimes \sum_i \kappa_i \hat{q}_i \equiv \underbrace{\hat{X}}_{\equiv \hat{S}} \otimes \hat{E}, \quad (4.26)$$

thus in our starting point (4.4) we get away with using only a single coupling term  $\alpha = 0$  and hence can drop the indices  $\alpha, \beta$ .

In order to assemble (4.21) we now need to calculate four pieces

- (i) The environmental self correlation functions  $\mathcal{C}(\tau)$ .
- (ii) The interaction picture evolution  $\hat{S}^{(I)}(\tau)$  of the system part of  $\hat{H}_{\text{int}}$ .
- (iii) The decoherence operators  $\hat{B}, \hat{C}$  [they follow from (i) and (ii)].
- (iv) The usual unitary system evolution  $[\hat{H}_S, \hat{\rho}_S(t)]$ .

#### 4.4.1 Environmental correlation functions and spectral densities

The correlation functions are defined in (4.15). Since we have only one environment operator in (4.26), namely  $\hat{E}$ , there are no indices  $\alpha, \beta$  (or they are both = 0). We thus require  $\mathcal{C}(\tau) = \text{Tr}_{\mathcal{E}} \left\{ \hat{E}^{(I)}(\tau) \hat{E}^{(I)}(0) \hat{\rho}_{\mathcal{E}}(0) \right\} = \langle \hat{E}^{(I)}(\tau) \hat{E}^{(I)}(0) \rangle_{\mathcal{E}}$ , where we have used (3.6). To evaluate this, we have to crucially assume a state  $\hat{\rho}_{\mathcal{E}}(0)$  for the environment. We pick the

**Thermal State for the Environment:** In analogy to what you know from thermodynamics, we can write the environmental density matrix in thermal equilibrium, with  $\beta = 1/k_B T$ , as

$$\hat{\rho}_{\mathcal{E}} = \frac{1}{Z} e^{-\beta \hat{H}_{\mathcal{E}}}, \quad Z = \text{Tr}[e^{-\beta \hat{H}_{\mathcal{E}}}] \quad (4.27)$$

Decomposed into individual oscillators, this becomes

$$\hat{\rho}_{\mathcal{E}} = \bigotimes_n \hat{\rho}_n = \bigotimes_n \left( \sum_k p_{kn} [|k\rangle\langle k|]_n \right), \quad p_{kn} = \frac{e^{-\beta \omega_k k}}{\sum_m e^{-\beta \omega_m m}}. \quad (4.28)$$

- Since we write (4.28) as a product of density matrices for each oscillator, the individual oscillators are uncorrelated. This means that all  $\langle \hat{O}_a \hat{O}_b \rangle = 0$  for  $a \neq b$ , where  $\hat{O}_a$  is an operator acting on oscillator  $a$  only (proof: exercise).
- We see that each possible state  $|k\rangle$  for an oscillator is occupied with probability given by the Boltzmann factor  $e^{-\beta E_k}$ , where  $E_k = \omega_k k$  is the energy of that state. The individual densities are mixed (see section 3.1.2).

We can now calculate the environmental correlation function. In a first step we note:

$$\mathcal{C}(\tau) \stackrel{\text{insert } \hat{E}}{=} \sum_{ij} \kappa_i \kappa_j \langle \hat{q}_i(\tau) \hat{q}_j(0) \rangle = \sum_j \kappa_j^2 \langle \hat{q}_j(\tau) \hat{q}_j(0) \rangle. \quad (4.29)$$

- The last step follows, because in (4.27) all the individual oscillators are uncorrelated.

In assignment 1 we have solved the interaction picture evolution for  $\hat{a}$ ,  $\hat{a}^\dagger$  (governed by  $\hat{H}_{\mathcal{E}}$  only), which allows us to use the inverse of (1.20) and write that of each oscillators position operator as:

$$\hat{q}_j(\tau) = \frac{1}{\sqrt{2m_j \omega_j}} (\hat{a}_j(0) e^{-i\omega_j \tau} + \hat{a}_j^\dagger(0) e^{i\omega_j \tau}). \quad (4.30)$$

Inserting (4.30) into (4.29) gives:

$$\mathcal{C}(\tau) = \sum_j \kappa_j^2 \left\{ \frac{1}{2m_j \omega_j} \left( \underbrace{\langle \hat{a}_j(0) \hat{a}_j^\dagger(0) \rangle}_{=\hat{a}_j^\dagger(0)\hat{a}_j(0)+1} e^{-i\omega_j \tau} + \underbrace{\langle \hat{a}_j^\dagger(0) \hat{a}_j(0) \rangle}_{\cos(\omega_j \tau) + i \sin(\omega_j \tau)} e^{i\omega_j \tau} \right) \right\} \quad (4.31)$$

In the state (4.28), we have the mean thermal occupation  $N_j(T) = \langle \hat{a}_j^\dagger(0) \hat{a}_j(0) \rangle = 1/(e^{\beta \omega_j} - 1)$  (exercise), and hence

$$\begin{aligned} \mathcal{C}(\tau) &= \sum_j \kappa_j^2 \left\{ \frac{1}{2m_j \omega_j} \left( [1 + 2N_j(T)] \cos(\omega_j \tau) - i \sin(\omega_j \tau) \right) \right\} \\ &= \sum_j \kappa_j^2 \left\{ \frac{1}{2m_j \omega_j} \left( \coth\left(\frac{\omega_j}{2k_B T}\right) \cos(\omega_j \tau) - i \sin(\omega_j \tau) \right) \right\} \\ &\equiv \nu(\tau) + i\eta(\tau). \end{aligned} \quad (4.32)$$

With the last line we have defined the

**Noise Kernel:**

$$\nu(\tau) = \sum_j \frac{\kappa_j^2}{2m_j\omega_j} \coth\left(\frac{\omega_j}{2k_B T}\right) \cos(\omega_j\tau) = \frac{1}{2} \sum_j \kappa_j^2 \langle \{\hat{q}_j(\tau), \hat{q}_j(0)\} \rangle \quad (4.33)$$

and **Dissipation Kernel:**

$$\eta(\tau) = \sum_j \frac{\kappa_j^2}{2m_j\omega_j} \sin(\omega_j\tau) = \frac{i}{2} \sum_j \kappa_j^2 \langle [\hat{q}_j(\tau), \hat{q}_j(0)] \rangle \quad (4.34)$$

- For the form using commutators you can re-follow the steps before (4.32).

Finally we define the

**Spectral Density:**

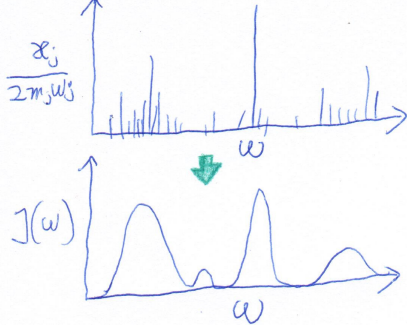
$$J(\omega) \equiv \sum_j \frac{\kappa_j^2}{2m_j\omega_j} \delta(\omega - \omega_j). \quad (4.35)$$

with which we can write

$$\begin{aligned} \nu(\tau) &= \int_0^\infty d\omega J(\omega) \coth\left(\frac{\omega}{2k_B T}\right) \cos(\omega\tau), \\ \eta(\tau) &= \int_0^\infty d\omega J(\omega) \sin(\omega\tau). \end{aligned} \quad (4.36)$$

- The reason for the Kernel names in (4.33) and (4.34) will become clear later.
- The influence of the environment onto the system in the Born Markov ME (4.21) is fully hidden in the environment correlations  $\mathcal{C}(\tau)$ . From the manipulations above we see that this in turn can be fully expressed via the spectral density of the environment.
- At zero temperature we have  $J(\omega) = \int_0^\infty d\omega \mathcal{C}(\tau) e^{-i\omega\tau}$ , so that the spectral density is the (half-sided) Fourier Transform of the environment correlation function  $\mathcal{C}(\tau)$ .

**Interpretation of spectral density:** The spectral density allows us to move from an explicitly numbered collection of environmental oscillators to a continuous distribution of them.



**left:** Consider the collection of oscillators on the left. We have drawn sticks of length  $L_j = \frac{\kappa_j^2}{2m_j\omega_j}$  at frequencies  $\omega_j$ . If there is a dense collection of sticks, their impact on the system will be well captured by  $J(\omega)$ .<sup>a</sup>

<sup>a</sup>In other words, any sum over sticks (4.33) or integral over  $J$  (4.36) for any small frequency interval  $\Delta\omega$  will be the same.

We have now completed item (i) of the list after Eq. (4.26).

#### 4.4.2 Assembling Master equation for Brownian motion

Proceeding further we require  $\hat{S}^{(I)}(\tau)$ , which in our case is  $\hat{X}^{(I)}(\tau)$ . Recall that an interaction picture operator evolves according to  $\hat{H}_0 = \hat{H}_S + \hat{H}_E$ , according to (1.41). From  $\hat{H}_S = \hat{P}^2/2M + M\Omega^2\hat{X}^2/2$  we find (still  $\hbar=1$ )

$$\begin{aligned} i\frac{\partial}{\partial t}\hat{X}_I(t) &= [\hat{X}_I(t), \hat{H}_{0I}(t)] = \frac{1}{M}i\hat{P}_I(t), \\ i\frac{\partial}{\partial t}\hat{P}_I(t) &= [\hat{P}_I(t), \hat{H}_{0I}(t)] = -iM\Omega^2\hat{X}_I(t). \end{aligned} \quad (4.37)$$

The second equalities above use that also  $[\hat{X}_I(t), \hat{P}_I(t)] = i\hbar$ , i.e. the commutation relations are preserved (this follows directly from (1.39)).

The equations (4.37) have the solution

$$\begin{aligned} \hat{X}_I(\tau) &= \hat{X}(0) \cos(\Omega\tau) + \frac{1}{M\Omega}\hat{P}(0) \sin(\Omega\tau), \\ \hat{P}_I(\tau) &= \hat{P}(0) \cos(\Omega\tau) - M\Omega\hat{X}(0) \sin(\Omega\tau). \end{aligned} \quad (4.38)$$

- Proof: Substitute (4.38) into (4.37).

Inserting  $\hat{S}^{(I)}(\tau) = \hat{X}_I(\tau)$  from (4.38) into (4.20) using (4.32) we obtain

$$\begin{aligned} \hat{B} &= \int_0^\infty d\tau \mathcal{C}(\tau)\hat{S}^{(I)}(-\tau) = \int_0^\infty d\tau (\nu(\tau) + i\eta(\tau)) \left( \hat{X}(0) \cos(-\Omega\tau) + \frac{1}{M\Omega}\hat{P}(0) \sin(-\Omega\tau) \right), \\ \hat{C} &= \int_0^\infty d\tau \mathcal{C}(-\tau)\hat{S}^{(I)}(-\tau) = \int_0^\infty d\tau (\nu(-\tau) + i\eta(-\tau)) \left( \hat{X}(0) \cos(-\Omega\tau) + \frac{1}{M\Omega}\hat{P}(0) \sin(-\Omega\tau) \right). \end{aligned} \quad (4.39)$$

In a final step we insert (4.39) into the general expression for a Born-Markov ME (4.21), then extensively re-arrange terms (exercise), to write the

**Master equation for Quantum Brownian Motion (QBM)**

$$\begin{aligned} \frac{d}{dt} \hat{\rho}_S(t) = & -i[\hat{H}_S + \frac{1}{2}M\tilde{\Omega}^2 \hat{X}^2, \hat{\rho}_S(t)] - i\gamma[\hat{X}, \{\hat{P}, \hat{\rho}_S(t)\}] \\ & - D[\hat{X}, [\hat{X}, \hat{\rho}_S(t)]] - f[\hat{X}, [\hat{P}, \hat{\rho}_S(t)]]. \end{aligned} \quad (4.40)$$

where all operators without time argument are at time  $t = 0$ . The coefficients are

$$\tilde{\Omega}^2 = -\frac{2}{M} \int_0^\infty d\tau \eta(\tau) \cos(\Omega\tau), \quad (4.41)$$

$$\gamma = \frac{1}{M\Omega} \int_0^\infty d\tau \eta(\tau) \sin(\Omega\tau), \quad (4.42)$$

$$D = \int_0^\infty d\tau \nu(\tau) \cos(\Omega\tau), \quad (4.43)$$

$$f = -\frac{1}{M\Omega} \int_0^\infty d\tau \nu(\tau) \sin(\Omega\tau). \quad (4.44)$$

- We have now achieved the goal to describe the central oscillator in terms of  $\hat{\rho}_S(t)$  and  $\hat{X}, \hat{P}$  only, even for a very large number of environmental oscillators.
- The time-evolution depends on constant coefficients  $\tilde{\Omega}^2, \gamma, D, f$ , that can fully be calculated from the original environmental coupling  $\kappa_j$ , frequency  $\omega_j$ , and state  $\hat{\rho}_E$ .

We will provide the physical meaning of the coefficients (4.41)-(4.44) in section 4.4.3. To that end, it will help to also look at (4.40) in the position basis. For this we first have to write the density matrix in the position basis as

$$\hat{\rho}_S = \int dX \int dX' \rho_S(X, X') |X\rangle \langle X'|. \quad (4.45)$$

Using further that that  $\langle X | \hat{P} \hat{\rho}_S | X' \rangle = -i \frac{\partial}{\partial X} \langle X | \hat{\rho}_S | X' \rangle$ , we then reach the

**QBM Master equation in position space**

$$\begin{aligned} \frac{d}{dt} \hat{\rho}_S(X, X', t) = & \left\{ -\frac{i}{2M} \left( \frac{\partial^2}{\partial X'^2} - \frac{\partial^2}{\partial X^2} \right) - \frac{i}{2}M(\Omega^2 + \tilde{\Omega}^2)(X^2 - X'^2) \right. \\ & + \gamma(X - X') \left( \frac{\partial}{\partial X'} - \frac{\partial}{\partial X} \right) - D(X - X')^2 \\ & \left. + i f(X - X') \left( \frac{\partial}{\partial X'} + \frac{\partial}{\partial X} \right) \right\} \rho_S(X, X', t). \end{aligned} \quad (4.46)$$

We now proceed to infer the consequences of all the "new terms" using both, (4.40) and (4.46).

### 4.4.3 Decoherence and Dissipation in Quantum Brownian motion

**part**  $\sim \tilde{\Omega}^2$ : The contribution by the  $\tilde{\Omega}^2$  term is easiest. It occurs in exactly the same place and way as the system oscillator frequency  $\Omega^2$ , and hence corresponds to an environmentally induced shift of the oscillator frequency. We had called that a Lamb shift in section 4.3.

**part**  $\sim \gamma$ : Consider the evolution of the mean momentum  $\langle \hat{P} \rangle$ , that follows from (4.40). We find that the  $\gamma$  term gives rise to

**Momentum damping or friction**, according to

$$\frac{d}{dt} \langle \hat{P} \rangle = -M(\Omega^2 + \tilde{\Omega}^2) \langle \hat{X} \rangle - 2\gamma \langle \hat{P} \rangle. \quad (4.47)$$

- The first term is just usually oscillatory motion in the Lamb-shifted oscillator potential.
- The second term alone would result in  $\langle \hat{P} \rangle = e^{-2\gamma t} \langle \hat{P} \rangle_{t=0}$ , i.e. exponential damping.

**Mean values from Master equation:** Deriving Eq. (4.47) is a good exercise. For example considering only the friction term  $\frac{d}{dt} \hat{\rho}_S(t) = \dots - i\gamma [\hat{X}, \{\hat{P}, \hat{\rho}_S(t)\}]$ , we can write

$$\begin{aligned} \frac{d}{dt} \langle \hat{P} \rangle &= \frac{d}{dt} \text{Tr}_{\mathcal{E}} \left\{ \hat{\rho}_S(t) \hat{P} \right\} = \text{Tr}_{\mathcal{E}} \left\{ \frac{d\hat{\rho}_S(t)}{dt} \hat{P} \right\} = -i\gamma \text{Tr}_{\mathcal{E}} \left\{ [\hat{X}, \{\hat{P}, \hat{\rho}_S(t)\}] \hat{P} \right\} \\ &= -i\gamma \text{Tr}_{\mathcal{E}} \left\{ \left( \hat{X}(\hat{P}\hat{\rho}_S(t) + \hat{\rho}_S(t)\hat{P}) - (\hat{P}\hat{\rho}_S(t) + \hat{\rho}_S(t)\hat{P})\hat{X} \right) \hat{P} \right\} \\ &= -i\gamma \text{Tr}_{\mathcal{E}} \left\{ \hat{\rho}_S(t) (\hat{P}\hat{X}\hat{P} + \underbrace{\hat{P}\hat{P}\hat{X} - \hat{X}\hat{P}\hat{P}}_{=[\hat{P}^2, \hat{X}] = -2i\hbar\hat{P}} - \hat{P}\hat{X}\hat{P}) \right\} = -i\gamma \text{Tr}_{\mathcal{E}} \left\{ \hat{\rho}_S(t) \hat{P} \right\} = -i\gamma \langle \hat{P} \rangle. \end{aligned} \quad (4.48)$$

- Exercise: Using similar steps, convince yourself that the D and f terms in (4.40) do not contribute to Eq. (4.47).
- Note that the friction coefficient  $\gamma$  depends only on the spectral density and not in temperature (only on  $\eta\tau$ , not on  $\nu(\tau)$ ).

**part**  $\sim D$ : This terms has two consequences. The first is best seen from (4.46), from where we infer the

### Spatial decoherence evolution

$$\frac{d}{dt}\hat{\rho}_S(X, X', t) = \dots - D(X - X')^2\rho_S(X, X', t), \quad (4.49)$$

which implies that spatial coherences in the reduced density matrix at a separation  $|X - X'|$  are decaying with a decoherence timescale  $\tau = 1/[D(X - X')^2]$ .

The second role can be seen by inspecting the

### Momentum diffusion

$$\frac{d}{dt}\langle\hat{P}^2\rangle = -M(\Omega^2 + \tilde{\Omega}^2)\langle\hat{X}\hat{P} + \hat{P}\hat{X}\rangle - 4\gamma\langle\hat{P}^2\rangle + 2D, \quad (4.50)$$

which means that just via the D-term, the variance of momentum<sup>a</sup> grows as  $\langle\hat{P}^2\rangle \sim Dt$ .  
 $\tau = 1/[D(X - X')^2]$ .

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<sup>a</sup>Assuming  $\langle\hat{P}\rangle = 0$ .

- $D$  is thus also referred to as normal diffusion coefficient
- The derivation of (4.50) is analogous to that of Eq. (4.47), see (4.48).
- Also position space uncertainty scales as  $\Delta X^2 \sim Dt$ .
- $D$  depends on the spectral density and on the temperature.

**part**  $\sim f$ : The  $f$  is called anomalous diffusion coefficient. It is usually much less important than the  $D$  coefficient. See SD for some more information.

#### 4.4.4 Types of spectral density, Ohmic Decoherence and Dissipation

The discussion of the previous section already contained all effects that occur for our oscillator in contact with the environment. Note, that for that we understood all these effects by only knowing the system part of the system-environment coupling  $\hat{S}^{(I)}(\tau) = \hat{X}_I(\tau)$ , the (operator) form of which then decides which terms occur in Eq. (4.40).

However to find out about the strength of these effects, i.e. value of the coefficients (4.41)-(4.44), we finally have to specify a spectral density. Often one does not take the path via the definition  $J(\omega) = \sum_j \frac{\kappa_j^2}{2m_j\omega_j} \delta(\omega - \omega_j)$ , for example because individual  $\kappa_j$  are not known. Instead one directly takes some of a frequently used

### List of spectral densities

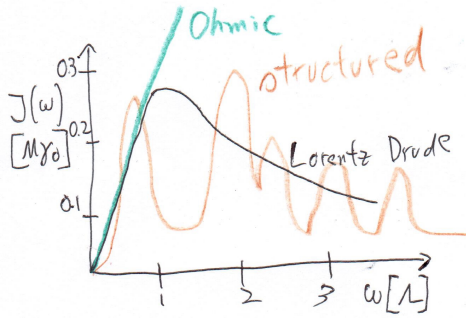
Ohmic spectral density:

$$J(\omega) = \frac{2M\gamma_0}{\pi}\omega. \quad (4.51)$$

Lorentz-Drude spectral density:

$$J(\omega) = \frac{2M\gamma_0}{\pi}\omega \frac{\Lambda^2}{\Lambda^2 + \omega^2}. \quad (4.52)$$

Structured spectral density: All the above have a very simple shape as seen below. Anything with more detail, such as multiple peaks, is called "structured spectral density".



**left:** Sketch of all the spectral densities discussed above. The Lorentz-Drude spectral density is the Ohmic one with a high frequency cut-off  $\Lambda$ .

We will focus now only on the Lorentz-Drude spectral density (4.52), which has the nice feature that all the coefficients in the previous section can be relatively easily evaluated.

We find

$$\gamma = \frac{2}{\pi} \frac{1}{M\Omega} J(\Omega) = \gamma_0 \frac{\Lambda^2}{\Lambda^2 + \Omega^2}, \quad (4.53)$$

$$D = \frac{2}{\pi} J(\Omega) \coth\left(\frac{\Omega}{2k_B T}\right) = M\gamma_0 \Omega \frac{\Lambda^2}{\Lambda^2 + \Omega^2} \coth\left(\frac{\Omega}{2k_B T}\right), \quad (4.54)$$

$$\tilde{\Omega}^2 = -2\gamma_0 \frac{\Lambda^3}{\Lambda^2 + \Omega^2}. \quad (4.55)$$

- We skipped  $f$ , it is not so important in this case.
- The first relation for  $\gamma$  and  $D$  is valid in general and expresses the coefficients via the spectral density evaluated at the frequency of the system oscillator. To see this for  $\gamma$  we gather its definition (4.42) and that of the dissipation Kernel  $\eta(\tau)$  (4.34) occurring in it, to see that  $\gamma$  is essentially the double Fourier sine-transform of the spectral density. This returns the original (odd) function.:  $\frac{2}{\pi} \int_0^\infty dk \sin(x'k) \int_0^\infty dx g(x) \sin(kx) = g(x')$ . Similarly, for  $D$  we use that the double cosine transform returns the original (even) function.
- Note that  $\gamma = \gamma_0$  for system frequencies below the cut-off ( $\Omega \ll \Lambda$ ), which is why we wrote it into  $J(\omega)$ .



- In the limit  $k_B T \gg \Omega$  (high temperatures) and  $\Omega \ll \Lambda$ , we can write  $D = 2M\gamma_0 k_B T$  and using the thermal de-Broglie wavelength for the system oscillator  $\lambda_{dB} = 1/\sqrt{2Mk_B T}$  the spatial decoherence time-scale  $\tau$  after (4.49) then becomes  $\tau^{-1} = \gamma_0 \left( \frac{X-X'}{\lambda_{dB}} \right)^2$ . This tells us that any spatial superpositions with an extent  $|X - X'|$  much larger than  $\lambda_{dB}$  will decohere much faster than the system dissipates (the rate for which is  $\gamma_0$ ).

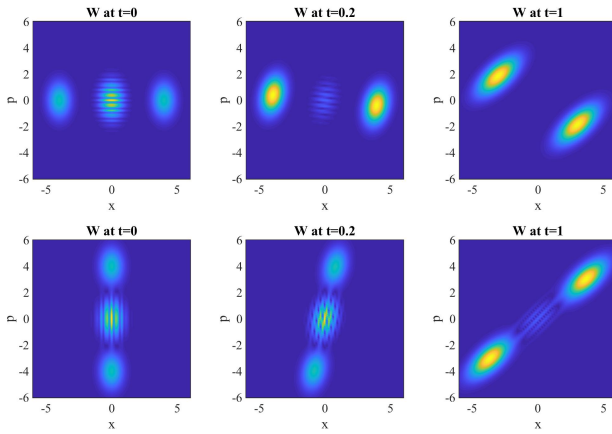
#### 4.4.5 Dynamics of Quantum Brownian motion

The previous discussion already allowed us to "guess" all physical effects relevant to QBM and their time-scales. However equations like (4.40) and (4.46) allow us to investigate the dynamics of these effects in much more detail.

**Numerical Quantum Brownian motion:** by a solution in position-space (of Eq. (4.46)). Let us consider two different (pure) initial states for our system oscillator

$$|\Psi_A(x)\rangle = \mathcal{N} \left( e^{-\frac{(x-x_0)^2}{2\sigma^2}} + e^{-\frac{(x+x_0)^2}{2\sigma^2}} \right), |\Psi_B(x)\rangle = \mathcal{N} e^{-\frac{x^2}{2\sigma^2}} \left( e^{ip_0 x/\hbar} + e^{-ip_0 x/\hbar} \right), \quad (4.56)$$

where  $|\Psi_A(x)\rangle$  is a superposition of two Gaussians in position space, and  $|\Psi_B(x)\rangle$  a superposition of two Gaussians in momentum space.



**left:** Evolution of the Wigner function (3.46) for the reduced density matrix  $\rho(x, x', t)$  evolving according to Eq. (4.46). The top row starts from the initial state  $|\Psi_A(x)\rangle$ , the bottom one from  $|\Psi_B(x)\rangle$ . We see that the interference features in the centre of phase space, indicating a superposition (see section 3.3.2) are damped out faster when starting in  $|\Psi_A(x)\rangle$ .

- We can use (4.46) including all the terms, to study for which density matrices the average decrease in purity (Eq. (3.10)) is smallest. Such states would be deemed most robust against decoherence. It turns out that these are precisely coherent states (1.26). In terms of our discussion in section 3.2.4, these would be the pointer states of the system.
- It makes sense that the spatial superposition  $|\Psi_A(x)\rangle$  in the example above decoheres faster than the momentum superposition  $|\Psi_B(x)\rangle$ . That is because the system part of  $\hat{H}_{\text{int}}$  is  $\hat{X}$ , thus the "environment measures X".