Heat transfer and entanglement – non-equilibrium correlation spectra of two quantum oscillators

Carsten Henkel

University of Potsdam, Institute of Physics and Astronomy,
Karl-Liebknecht-Str. 24/25, 14476 Potsdam, Germany
Email Address: henkel@uni-potsdam.de

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The non-equilibrium state of two oscillators with a mutual interaction and coupled to separate heat baths is discussed. Bosonic baths are considered, and an exact spectral representation for the elements of the covariance matrix is provided analytically. A wide class of spectral densities for the relevant bath modes is allowed for. The validity of the fluctuation-dissipation theorem is established for global equilibrium (both baths at the same temperature) in the stationary state. Spectral measures of entanglement are suggested by comparing to the equilibrium spectrum of zero-point fluctuations. No rotating-wave approximation is applied, and anomalous heat transport from cold to hot bath, as reported in earlier work, is demonstrated not to occur.

1 Introduction

The advent of quantum technology has triggered a re-analysis of thermodynamic concepts, producing many examples of deviations and anomalies. The intimate connection between a system state and information about it that is characteristic for quantum physics, has provided the basis for engines that transform information into work [1]. The thermodynamic viewpoint has also revigorated interest in open quantum systems, in contact with a bath and being monitored, possibly continuously. The dynamics of open quantum systems was traditionally formulated with the help of master equations [2] or influence functionals [3]. We are witnessing a renewed discussion about the details how these equations of motion should be set up, in order to respect basic requirements of both thermodynamics and quantum mechanics [4, 5, 6]. A system coupled to two different heat baths provides a paradigmatic example: it can be used to study heat transport, but also leads to interesting non-equilibrium states. In the presence of strong coupling to a bath, the separation, e.g. in terms of energy, between system and bath gets blurred. It is no longer obvious that a given dynamical model (master equation, Langevin equation) should be judged by its ability to generate the stationary system state that is expected from the Boltzmann-Gibbs canonical ensemble for the isolated system. After all, energy levels are being broadened and shifted by the contact with the bath, so that a careful procedure of removing the contact to the bath should be applied. The typical assumptions for baths used in deriving master equations actually complicate the situation: a continuous set of oscillators is by itself unable to thermalise, for example, and a bath in a thermal equilibrium state has to be specified by its initial conditions. In this context, master equations cannot, in general, be in Markov form because of memory kernels whose characteristic time constants are set by the spectral density of the bath modes in so far they couple to the system.
The background for the present study is provided by two contributions. Dorofeyev [7] has given for a system of two coupled oscillators coupled to bosonic baths a spectral representation of the interaction energy. This spectrum provides a way to visualise the heat flow across the two normal modes of the coupled oscillators. Levy and Kosloff [8] proposed a very similar model and showed that the parameters of the two-oscillator system can be such that heat is flowing from cold to hot, in stark violation of the second law. This has been taken as indication that one should abandon the concept of “local coupling” to a bath (each oscillator couples to its “own bath”, not correlated with the bath coupled to the other one), and replace it by a “global” approach where the two oscillators are considered as a one system first. In the aftermath of this paper, the issue of “local” vs. “global” couplings has been tested on various systems [5, 9, 10, 11, 12, 13, 14].

A related question arises in the interplay with dissipation on the one hand, as described by a master equation in Lindblad form, and additional interactions on the other, that may be added to the Hamiltonian part of the master equation [6]. The problem is also rooted in memory effects [15, 16, 17], in particular when the bath has a structured spectrum and the precise values of Bohr frequencies are relevant, as these are shifted either by the bath or by additional interactions. Complications then arise with respect to the order in which the secular and the Markov approximations are applied [6]. It has been argued that the Markov approximation behind some master equations is to blame. The advantage of the quantum Langevin formalism used here is that it is naturally non-Markovian, as soon as the memory kernels are of nonzero range – which is, of course, the generic case.

We study here an extremely simple situation that permits calculations with no approximations and avoids a few of the delicate issues mentioned before. We revisit the two coupled oscillators studied by Dorofeyev and Levy and Kosloff, but use a slightly different coupling that preserves positivity of the Hamiltonian and is not restricted to near-degenerate resonance frequencies,

\[ V = \frac{\lambda}{2} (x - y)^2 \]  

where \( x, y \) are the oscillator coordinates. The Heisenberg equations of motion are worked out and take the form of exact quantum Langevin equations [18]. For this non-Markovian system out of thermal equilibrium, we compute the covariance matrix of the position and momentum canonical coordinates (also known as continuous variables in quantum information). The formalism easily affords us with spectral representations of two-time correlations in the long-time limit. The heat current flowing through the system can be found by an energy balance argument, very similar to Dorofeyev’s analysis. We find that it is always directed from the hot to the cold bath, under very general assumptions. (The baths may have any spectral density, the damping kernels may have any memory, the bath-induced friction may be strong or weak compared to the interaction between oscillators.) The anomalous heat current of Levy & Kosloff [8] thus appears to be an artefact of the rotating-wave approximation made in the interaction

\[ V = \epsilon (a^\dagger b + ab^\dagger) = \lambda xy + \lambda' p_x p_y \]  

where \( a, b \) are the bosonic lowering operators constructed from \( x \) and \( y \) and their conjugate momenta and \( \lambda, \lambda' \propto \epsilon \). As an additional check of the consistency of the results, we consider equilibrium conditions with both baths having the same temperature, other parameters remaining arbitrary. The two-oscillator system then reaches a state where its two-time correlation functions satisfy
the fluctuation–dissipation theorem. The quantum Langevin model thus relaxes the system (whatever the initial conditions) towards thermal equilibrium at long times. The correlation functions in this equilibrium state differ from those obtained for a canonical density operator \( \exp(-H_{12}/T)/Z \) because of bath-induced friction, a well-known feature of the fluctuation–dissipation theorem for strongly damped systems [18, 19, 20]. The Boltzmann–Gibbs state might be reached by disconnecting the baths (weak-coupling regime), although even that requires some “decoupling work” to be done [4].

In a second step, we consider entanglement measures computed from the covariance matrix at large times. We point out that the criterion of a positive partially transposed covariance matrix may be used to construct a pair of canonical coordinates whose variances apparently drop below the Heisenberg limit, in close analogy to the large-distance correlations analysed by Einstein, Podolsky, and Rosen [21]. This construction can be carried over to the spectral domain, using techniques similar to those introduced by Ekstein and Rostoker [22] and familiar in filter theory (in the sense of Wagner and Campbell for signal processing [23, 24]). We can thus formulate a protocol that identifies the frequency band where the non-classical correlations (entanglement) between the two oscillators can be detected with the best margin.

2 Model

2.1 Hamiltonian

For completeness, we spell out in this section the Hamiltonian of the system. Readers familiar with the Langevin equation may jump directly to Sec. 2.2.

The two oscillators are described by the Hamiltonian [7, 25]

\[
H_{12} = \frac{p_x^2}{2m_1} + \frac{k_1}{2} x^2 + \frac{p_y^2}{2m_2} + \frac{k_2}{2} y^2 + \frac{1}{2} \lambda (x - y)^2
\]

with the bilinear interaction \( V_m(x - y) \) of Eq. (1). The obvious notation is based on mechanical oscillators with displacements \( x, y \), but the model can be re-framed easily to electric systems like an LC circuit

\[
\Phi^2 \quad \text{with} \quad \frac{\Phi^2}{2L} + \frac{C}{2} Q^2
\]

where \( Q \) is the charge on a capacity with capacitance \( C > 0, \Phi = L\dot{Q} \) the magnetic flux, and \( L > 0 \) the circuit (self-)inductance. In this language, the coupling \( V_m \) in Eq. (3) would be called capacitive. The canonical commutator \([\Phi, Q] = i\hbar\) then yields the magnetic flux quantum \( \hbar/e \).

Each oscillator is coupled to a bosonic bath, i.e. a collection of oscillators

\[
H_{B1} = \sum_{j \in B1} \left( \frac{p_j^2}{2m_j} + \frac{k_j}{2} (q_j - c_j x)^2 \right)
\]

where \( c_j \) is a (dimensionless) coupling constant and B1 represents the bath modes. For one oscillator, this would correspond to the Ullersma [26] or Caldeira–Leggett [27] model. The dynamics
becomes irreversible if we go to the continuum limit where the spectral density
\[
\rho_1(\omega) = \frac{\pi}{2} \sum_{j \in B_1} k_j c_j^2 \delta(\omega - \omega_j)
\]  
(5)
with \(\omega_j^2 = k_j/m_j\) becomes a smooth function. (This definition of the spectral density for the oscillator-bath coupling follows the convention of Ref. [7].) We assume that the spring constants \(k_j\) and couplings \(c_j\) are such that \(\rho_1(\omega)\) smoothly decays to zero in the UV. (For this reason, \(\rho_1(\omega)\) differs from the bath density of states by more than just some power of the frequency.) We fix an initial time \(t = 0\) where the bath coordinates have equilibrated with the (‘clamped’) positions \(x(0)\) and \(y(0)\) of the oscillators. This leads to the correlations
\[
\langle p_j(0) \rangle_T = 0 = \langle q_j(0) - x(0) \rangle_T
\]  
(6)
where \(\langle \ldots \rangle_T\) denotes the average at the bath temperature. Defining the symmetrised covariances for any two bath operators
\[
\langle A, B \rangle_T := \frac{1}{2} \langle AB + BA \rangle_T - \langle A \rangle_T \langle B \rangle_T
\]  
(7)
their values in thermal equilibrium take the form
\[
\frac{k_j}{2} \langle q_j, q_j \rangle_T = \frac{k_j}{2} \langle [q_j - x(0)]^2 \rangle_T = \frac{1}{2} \vartheta(\omega_j),
\]
\[
\frac{\langle p_j, p_j \rangle_T}{2m_j} = \frac{1}{2} \vartheta(\omega_j)
\]  
(8)
The mixed symmetrised correlation \(\langle q_j, p_k \rangle_T\) vanishes, and different normal modes \(j \neq k\) are not correlated: \(\langle q_j, q_k \rangle_T = 0 = \langle p_j, p_k \rangle_T\). Here, the effective temperature is (we set the Boltzmann constant \(k_B = 1\))
\[
\vartheta(\omega) = \frac{\hbar \omega}{2} \coth \frac{\hbar \omega}{2T} = \hbar \omega \left[ \bar{n}(\omega) + \frac{1}{2} \right]
\]  
(9)
where \(\bar{n}(\omega)\) is the Bose-Einstein distribution and \(\frac{1}{2} \hbar \omega\) the zero-point energy. In the high-temperature (or low-frequency) limit, \(\vartheta(\omega)\) reaches the classical (equipartition) value \(T\). By averaging the commutator \(\langle [q_j, p_j] = q_j p_j - p_j q_j = i\hbar \rangle\), one gets the non-symmetric correlations
\[
\langle (q_j - x(0)) p_j \rangle_T = -\langle p_j (q_j - x(0)) \rangle_T = \frac{i\hbar}{2}
\]  
(10)
Similar expressions describe the bath attached to the other oscillator; its spectral density will be denoted \(\rho_2(\omega)\). If the baths have different temperatures \(T_2 \neq T_1\), this allows for a nonzero heat current. The key assumption of this model is that the initial conditions for the dynamical variables of bath 1 and bath 2 show no cross-correlations (‘local bath’).

### 2.2 Langevin equations

The elimination of the bath coordinates outlined in Appendix A.1 leads to the pair of Langevin equations
\[
\dot{p}_x + k_1' x = \lambda y - \mu_1 \dot{x} + F_1(t)
\]  
(11)
\[
\dot{p}_y + k_2' y = \lambda x - \mu_2 \dot{y} + F_2(t)
\]  
(12)
Here, we recognise with the spring constant \( \lambda \) the force exerted mutually by the oscillators. It also modifies the oscillators’ spring constants according to \( k_i' = k_i + \lambda (i = 1, 2) \). The friction force \( \mu_1 \dot{x} \) is the convolution
\[
(\mu_1 \dot{x})(t) = \int \! d\tau \, \mu_1(\tau)\dot{x}(t - \tau) \tag{13}
\]
(analogously for \( \mu_2 \dot{y} \)), and its kernel \( \mu_1(\tau) \) given by
\[
\mu_1(\tau) = \Theta(\tau) \int_0^\infty \! \frac{d\omega}{\pi/2} \rho_1(\omega) \cos \omega \tau \tag{14}
\]
The friction force is causal so that only past values \( t - \tau \leq t \) of the velocity are contributing. The familiar Ohmic (memoryless) case corresponds to \( \rho_1(\omega) = \Gamma_1 \) with the usual friction coefficient \( \Gamma_1 \), since in this limit, \( \mu_1 \dot{x} = \Gamma_1 \dot{x} \). (The step function \( \Theta(\tau) \) cuts off one half of the \( \delta(\tau) \).) Defining the Fourier transform by
\[
\mu_i(\omega) = \int \! d\tau \, e^{i\omega \tau} \mu_i(\tau) \tag{15}
\]
we note the relation
\[
\text{Re} \, \mu_i(\omega) = \rho_i(\omega). \tag{16}
\]
This strictly holds only for \( \omega > 0 \), but since \( \mu_i(\omega) \) describes a response between real quantities, \( \text{Re} \, \mu_i(\omega) \) is an even function along the real axis. It is thus convenient to consider \( \rho_i(\omega) \) even in \( \omega \). Furthermore, \( \mu_i(\tau) \) being a causal kernel (vanishing for \( \tau < 0 \)), its Fourier transform is analytic in the upper half of the complex frequency plane (Titchmarsh theorem, Kramers–Kronig relations).

The Langevin force \( F_1(t) \) vanishes on average and its autocorrelation function has a similar representation in terms of the bath spectrum
\[
\langle F_1(t), F_1(t') \rangle_1 = \frac{\hbar}{2} \int_0^\infty \! \frac{d\omega}{\pi/2} \rho_1(\omega) \omega \coth \frac{\hbar \omega}{2T_1} \cos \omega(t' - t) \tag{17}
\]
Here, \( \langle \ldots \rangle_1 \) denotes the average with respect to the temperature of bath 1. The effective temperature \( \vartheta(\omega) \) defined in Eq. (9) is thus evaluated with \( T_1 \). The Fourier transformed Langevin force will be used in Sec. 3 to generate averages and correlation spectra. This is somewhat symbolic since \( F_1(\omega) \) does not exist in the conventional sense. By taking the double Fourier transform of the force-force correlation function, we get, however
\[
\langle F_1^*(\omega), F_1(\omega') \rangle_1 = \int \! dt \, dt' \, e^{i(\omega't' - \omega t)} \langle F_1(t), F_1(t') \rangle
\]
\[
= 2\pi \delta(\omega' - \omega) \int \! d\tau \, e^{i\omega \tau} \langle F_1(t), F_1(t + \tau) \rangle_1
\]
\[
= \pi \delta(\omega' - \omega) \rho_1(\omega) \tag{18}
\]
since the bath correlations are stationary and depend only on the time difference. (At this point, we consider \( t \) and \( t' \) to be in the late future of the initial time.) The \( \tau \)-integral over the correlation function exists and defines the spectral density \( S_{F_1}(\omega) \) of the Langevin force (Wiener-Khintchine theorem [28]). Since this correlation function is real and even, the same is true for the spectral density, and we get by comparison to Eq. (17)
\[
S_{F_1}(\omega) = 4\rho_1(\omega) \vartheta_1(\omega) \tag{19}
\]
2.3 Remarks

which is the fluctuation–dissipation relation for the Langevin force [3]. The prefactors in Eq. (18, 19) arise from the convention that $S_F$ represents the force autocorrelation by an integral over positive frequencies only [see Eq. (17)].

Analogous formulas apply for the Langevin force $F_2(t)$. The assumption that each oscillator couples to its local bath implies that there are no cross-correlations $\langle F_1(t), F_2(t') \rangle = 0$.

2.3 Remarks

The Langevin forces $F_1(t), F_2(t)$ are defined in such a way that they depend on the initial conditions of the baths whose joint state is assumed to factorise. As the system evolves, however, correlations arise among the two baths due to the coupling $\lambda$ between the oscillators. Similarly, the friction forces arise because the attached oscillators ‘polarise’ their baths [the inhomogeneous term in Eq. (66)]. These features are used in input-output theory [29] to analyse the information about the system made available in the bath variables (rather than ignoring these as unobservable).

We already mentioned the simple Ohmic case of memoryless friction, but this is does not necessarily imply a white noise spectrum for the Langevin force. Indeed, only in the high-temperature (low-frequency, or classical) limit does the force spectrum have the same frequency scaling as the friction kernel, as is also apparent from the fluctuation–dissipation relation (19). In particular in the quantum limit $\coth(\hbar \omega/2T) \to \text{sign}(\omega)$, the quantum noise spectrum is potentially wider. The coupling constants $c_j$ then play an essential role in determining the bath correlation time – the latter is notably set by the width of the relevant mode spectrum that actually couples to the system.

Dorofeyev [7] and Ghesquièere et al. [30] choose the interaction in the bilinear form $-\lambda xy$ and have to deal with instabilities at couplings $\lambda^2 \geq k_1 k_2$ where the potential surface becomes a saddle and the system can escape to infinity along the directions $x = y$ in the $xy$-plane. This is avoided with the positive definite interaction (1), the price to pay being the shift $k_i' = k_i + \lambda$ in the oscillator spring constants. The stability condition $\lambda^2 < k_1' k_2'$ then holds for any positive spring constant $\lambda$ (and even for $0 \geq \lambda > -k_1 k_2/(k_1 + k_2)$).

3 Correlation spectra

3.1 Representation in Fourier space

In this section, we solve the Langevin equations (11, 12) by a Fourier transformation and compute expectation values. Since the friction kernels are in convolution form, we find

$$
\begin{pmatrix}
K_1(\omega) & -\lambda \\
-\lambda & K_2(\omega)
\end{pmatrix}
\begin{pmatrix}
x(\omega) \\
y(\omega)
\end{pmatrix} =
\begin{pmatrix}
F_1(\omega) \\
F_2(\omega)
\end{pmatrix}
$$

(20)

Here, the diagonal terms (we may call them inverse susceptibilities) are

$$
K_1(\omega) = -m_1 \omega^2 - i \omega \mu_1(\omega) + k_1'
$$

(21)

and $\mu_1(\omega)$ is the Fourier transform of the friction kernel (14).
The solution of the linear system (20) is immediate
\[
\begin{pmatrix}
  x(\omega) \\
  y(\omega)
\end{pmatrix} = \frac{1}{D(\omega)} \begin{pmatrix}
  K_2(\omega) & \lambda \\
  \lambda & K_1(\omega)
\end{pmatrix} \begin{pmatrix}
  F_1(\omega) \\
  F_2(\omega)
\end{pmatrix}
\]  
(22)
and involves the determinant
\[
D(\omega) = K_1(\omega)K_2(\omega) - \lambda^2
\]  
(23)
Its zeros determine the eigenmodes of the coupled oscillator system. In the simple case that damping is negligible, one gets
\[
\omega_{\pm}^2 \approx \frac{\omega_1^2 + \omega_2^2}{2} \pm \frac{1}{2} \left[ (\omega_1^2 - \omega_2^2)^2 + 4g^4 \right]^{1/2}
\]  
(24)
where \(\omega_i^2 = k_i/m_i \) \((i = 1, 2)\) are the eigenfrequencies. They are shifted and pushed apart by the coupling \(g^2 = \lambda/\sqrt{m_1 m_2}\). Another simple case where the fourth-order characteristic polynomial simplifies is the near-resonant one \(\omega \sim \omega_{1,2}\) where the rotating-wave approximation can be applied. The susceptibilities are then linearised, \(K_1(\omega) \approx 2m_1\omega_1(\omega_1 - i\gamma_1/2 - \omega)\) with \(\gamma_1 = \mu_1(\omega_1)/m_1\). The secular frequencies are found as
\[
\omega_{\pm} \approx \frac{\Omega_1 + \Omega_2}{2} \pm \frac{1}{2} \left[ (\Omega_1 - \Omega_2)^2 + g_r^2 \right]^{1/2}
\]  
(25)
with the complex bare resonances \(\Omega_1 = \omega_1 - i\gamma_1/2\) and the effective coupling \(g_r = \lambda/\sqrt{m_1 m_2}\omega_1\omega_2\). In particular in optical spectroscopy, one speaks of a strongly coupled system when \(g_r\) exceeds the linewidths \(\Re(\gamma_1 + \gamma_2)\) so that the complex resonances \(\omega_{\pm}\) are well-resolved. The near-resonant approximation neglects the spectral structure of the bath (and the concomitant memory effects) by evaluating \(\mu_1(\omega_1)\) at the resonance frequency. A more complete evaluation would lead to shifted and additional poles.

This behaviour is illustrated in Fig. 1. We consider a typical setting of “absorption spectroscopy” where two external monochromatic forces with amplitudes \(f_1, f_2\) and frequency \(\omega\) perturb the two oscillators. This drives the oscillators out of equilibrium, but the external energy is eventually dumped into the baths. In the long-time limit, the total absorbed power is given by (for more details, see Sec. 3.4)
\[
\langle \dot{x} \rangle f_1 + \langle \dot{y} \rangle f_2 = \omega |f_1|^2 \Im \frac{K_2(\omega)}{D(\omega)} + \omega |f_2|^2 \Im \frac{K_1(\omega)}{D(\omega)}
\]  
(26)
where the overline denotes the time average. The imaginary part \(\omega \Im[K_2(\omega)/D(\omega)]\) can also be interpreted as the spectral function (effective mode density) for the oscillator 1. The dotted lines in the Figure correspond to the non-coupled oscillators where \(\omega \Im[1/K_1(\omega)]\) peaks. The vertical solid lines give the normal mode frequencies \(\omega_{\pm}\) [Eq. (24)]. For detuned oscillators, the absorption spectra show a peak and a shoulder at the eigenfrequencies [panel (a)]. At critical coupling, the normal mode splitting is barely larger than the oscillators’ linewidths [panel (b)]. A colored bath [panel (c), see Eq. (27)] shifts the absorption peaks significantly relative to the prediction (24).

In the preceding plots, we consider a memory kernel with a Drude regularisation. It corresponds to the spectral density
\[
\rho(\omega) = \frac{\gamma/\tau_c^2}{\omega^2 + 1/\tau_c^2}
\]  
(27)
3.2 Stationary covariances

From the Fourier relation (22), we can construct the stationary behavior of the coupled oscillators. One remarks first of all that the poles of the response matrix that define the eigenfrequencies of the system, are located below the real axis so that the system loses the memory of its initial conditions (damped oscillator). (The same would be true for poles that coalesce into branch cuts for certain spectral densities.) The mean values of the phase space coordinates \((x, p_x, y, p_y)\) thus vanish on time scales larger than \(\sim 1/\Re \mu_i(\omega_i)\). The same result is obtained by taking the mean value of Eq. (22), since the Langevin forces vanish on average.

In the following, we focus on the fluctuations around these mean values. They are captured by the covariance matrix defined by analogy to Eq. (7):

\[
C_{ij} = \lim_{t \to \infty} \langle q_i(t), q_j(t) \rangle_{12}, \quad (q_i) = (x, p_x, y, p_y)^T
\]

(28)

where the double index 12 reminds that the baths coupled to the two oscillators are taken in equilibrium at temperatures \(T_1\) and \(T_2\).
3.3 Crossed correlations

We illustrate the calculation with the difference coordinate studied by Dorofeyev [7] because it determines the average interaction energy. The Fourier solution yields

\[ x(\omega) - y(\omega) = \frac{K_2(\omega) - \lambda}{D(\omega)} F_1(\omega) - \frac{K_1(\omega) - \lambda}{D(\omega)} F_2(\omega) \]  

(29)

When we compute the average \( \langle (x(t) - y(t))^2 \rangle_{12} \) from the Fourier transform (29), the fact (18) that different frequencies are not correlated, implies that the average is stationary. We thus drop the time argument and find

\[ \langle (x - y)^2 \rangle_{12} = \int_0^\infty d\omega \frac{2\pi}{2\pi} \left\{ \left| \frac{K_2(\omega) - \lambda}{D(\omega)} \right|^2 S_{F_1}(\omega) + \left| \frac{K_1(\omega) - \lambda}{D(\omega)} \right|^2 S_{F_2}(\omega) \right\} \]  

(30)

It can be checked that this formula agrees with Eqs.(12–14) of Ref. [7] where the covariance \(-\lambda \langle x, y \rangle_{12}\) is given separately (mean interaction energy). By similar calculations, we get the diagonal element of the covariance matrix (28)

\[ C_{xx} = \int_0^\infty d\omega \frac{2\pi}{4\pi} e^{i\omega(t-t')} \sum_i \alpha_i^*(\omega) \beta_i(\omega) S_{F_i}(\omega) \]  

(31)

and an analogous result for \( C_{yy} \). We see here how the thermal spectrum of bath 2 couples to the oscillator position fluctuations; this second term in Eq. (31) is naturally proportional to the oscillator coupling \( \lambda \). The mixed position-momentum \( C_{xp} \) covariance vanishes. This result and the expression for the mixed correlation \( C_{xp_y} \) between the oscillators are discussed next.

3.3 Crossed correlations

One key insight of the quantum Langevin model [7] is that without much further effort, the preceding results also provide the two-time correlation functions of the oscillator fluctuations in the stationary state. This state is not in thermal equilibrium: due to the difference in bath temperatures, there is actually a heat current flowing through the system. The cross-correlation functions thus provide insight into the dynamical aspects of deviations from a local equilibrium state.

We start with a general expression for a two-time correlation between observables \( A \) and \( B \)

\[ \langle A(t), B(t') \rangle_{12} = \int \frac{d\omega}{2\pi} \frac{d\omega'}{2\pi} e^{i(\omega t - \omega' t')} \sum_{ij} \alpha_i^*(\omega) \beta_j(\omega') \langle F_i(\omega), F_j(\omega') \rangle_{12} \]

\[ = \int \frac{d\omega}{4\pi} e^{i\omega(t-t')} \sum_i \alpha_i^*(\omega) \beta_i(\omega) S_{F_i}(\omega) \]  

(32)

Here, the functions \( \alpha_i(\omega) \) and \( \beta_i(\omega) \) provide the response of the observables \( A \) and \( B \) to the Langevin forces \( F_i \) of the baths, \( A(\omega) = \alpha_1(\omega) F_1(\omega) + \alpha_2(\omega) F_2(\omega) \). In the second line, the bath spectral
3.4 Heat current spectrum

densities $S_{Fi}(\omega)$ from Eq. (18) are used. From Eq. (19), they are symmetric in $\omega$ so that positive and negative frequencies can be combined. In this step, the identities $\alpha_i^*(\omega) = \alpha_i(-\omega)$ are useful which must hold for a hermitean observable $A(t)$. This leads to the following convention for the cross-correlation spectrum $S_{AB}(\omega)$ (in general a complex quantity)

$$
\langle A(t), B(t') \rangle_{12} = \int_0^\infty \frac{d\omega}{2\pi} \text{Re} \left[ e^{i\omega(t-t')} S_{AB}(\omega) \right]
$$

$$
S_{AB}(\omega) = \sum_i \alpha_i^*(\omega) \beta_i(\omega) S_{Fi}(\omega)
$$

As an example, consider the pair $(A, B) = (x, p_x)$. We can read off $\alpha_i(\omega)$ ($i = 1, 2$) from the first line of the linear response matrix (22). In addition, from $p_x = m_1 \dot{x}$ follows the simple relation $\beta_i(\omega) = -im_1 \omega \alpha_i(\omega)$. The correlation spectrum becomes

$$
S_{xp_x}(\omega) = -im_1 \omega |K_2|^2 S_{F1} + \lambda^2 S_{F2} \over |D|^2
$$

where the frequency arguments are suppressed for simplicity. This is purely imaginary and therefore, the equal-time correlation $\langle x, p_x \rangle$ vanishes.

The results for the cross-covariance matrix can be collected into a matrix (boldface for $2 \times 2$-matrices)

$$
C(t - t') = \begin{pmatrix}
\langle x(t), y(t') \rangle_{12} & \langle x(t), p_y(t') \rangle_{12} \\
\langle p_x(t), y(t') \rangle_{12} & \langle p_x(t), p_y(t') \rangle_{12}
\end{pmatrix}
$$

and have the following cross-correlation spectra

$$
\begin{pmatrix}
S_{xy} & S_{xp_y} \\
S_{px_y} & S_{pp_y}
\end{pmatrix} = \lambda \begin{pmatrix}
1 & -im_2 \omega \\
im_1 \omega & m_1 m_2 \omega^2
\end{pmatrix} \frac{K_2^* S_{F1} + K_1 S_{F2}}{|D|^2}
$$

The last fraction becomes real in the case of equal temperatures because Eq. (16) yields

$$
i \omega [\mu_2^* \rho_1 - \mu_1 \rho_2] = \text{Im}(\mu_2) \rho_1 + \text{Im}(\mu_1) \rho_2
$$

so that the mixed position-momentum correlations vanish at equal times, $\langle x, p_y \rangle_{12} = 0 = \langle p_x, y \rangle$.

3.4 Heat current spectrum

The correlation function $\langle x(t), p_y(t') \rangle$ actually captures the heat current through the link between the oscillators. To see this, we calculate the power exchanged by oscillators and heat baths (see Fig. 2). It follows from the time-averaged derivative of the energy of the (isolated) oscillator $(x, p_x)$

$$
\langle \frac{dH_1}{dt} \rangle = \lambda \langle \dot{x}(y - x) \rangle - \langle \dot{x}(\mu_1 * \dot{x}) \rangle + \langle F_1 \dot{x} \rangle
$$

The first term is the power transferred by the connecting spring. The second term is negative definite (for any friction kernel) and can be interpreted as the power dissipated into heat bath 1. Finally, the last term is the rate of work performed by the Langevin force $F_1$ on the oscillator $(x, p_x)$. 

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3.4 Heat current spectrum

These assignments of energy fluxes are illustrated in Fig. 2. We have used that \( \langle \dot{x}x \rangle = 0 \) and \( \langle \dot{x}y \rangle + \langle \dot{y}x \rangle = 0 \) in a stationary state to re-write the power exchanged by the oscillators in a more “anti-symmetric” way. The energy balance illustrates why the absorption spectrum defined in Eq. (26) is equivalent to the power dissipated into the bath (in linear response to the perturbing fields). In the stationary state, it justifies that the heat current from bath 1 to bath 2 across the two oscillators can be computed as [31]

\[
\dot{Q}_{1\rightarrow 2} = \frac{\lambda}{2} \langle \dot{x}y - \dot{y}x \rangle
\]

(40)

(Any other point in the chain would give the same value, of course.) In the stationary state, we identify this with the correlation function \( \langle x, p \rangle_{12}/m_2 - \langle p, y \rangle_{12}/m_1 \) and get from Eq. (37) the following spectral representation:

\[
\dot{Q}_{1\rightarrow 2} = \lambda^2 \int_0^\infty \frac{d\omega}{2\pi} \frac{S_{F1} \text{Im} K_2 - S_{F2} \text{Im} K_1}{|D|^2}
\]

This simplifies with Eqs.(19, 21) to

\[
\dot{Q}_{1\rightarrow 2} = 4\lambda^2 \int_0^\infty \frac{d\omega}{2\pi} \omega^2 \rho_1 \rho_2 |D|^2 (\bar{\vartheta}_1 - \bar{\vartheta}_2)
\]

(42)

where the relation (16) between damping kernel and spectral density was used. The net heat current vanishes when both baths are at the same temperature, and heat flows from the hot to the cold bath because the spectral densities \( \rho_i(\omega) \) are non-negative.

The heat current spectrum is illustrated in Fig. 3. On the left, we consider a differential heat gradient \( T_1 = T_2 + dT \) where \( \vartheta_1(\omega) - \vartheta_2(\omega) = dT(\hbar \omega/T)^2 \bar{n}(\bar{n} + 1) \) with the Bose-Einstein distribution \( \bar{n} = \bar{n}(\omega) \) evaluated at the mean bath temperature \( T \). We plot the dimensionless quantity \( d\dot{Q}_{12}/dT df \) which is defined as the integrand of Eq. (42) \( (df = d\omega/2\pi) \). For detuned oscillators, the eigenfrequencies define peaks of efficient heat transport [Fig. 3(left), case (a)]. Note that in the critical coupling scenario (b), only one peak is visible because the splitting of the normal modes is still comparable to the linewidth. Strong coupling separates the two channels in frequency [case (c)]. When comparing to the absorption spectrum of Fig. 1, it is interesting that the latter is larger in case (a), although the heat current stays relatively weak. This may be attributed to the small overlap between the two resonances.

Figure 2: Illustration of power exchanged between oscillators and baths. The net heat current is given by the difference \( \dot{Q}_{1\rightarrow 2} = \frac{1}{2} \lambda \langle x\dot{y} - \dot{x}y \rangle_{12} \) where the average is taken in the non-equilibrium stationary state, assuming two different temperatures for the heat baths.
The motivation for Fig. 3(right) with a finite temperature difference $\Delta T = T_1 - T_2$ is the comparison to Levy & Kosloff [8]. The heat current given by Eq. (42) is one of the main results of the present paper because Clausius’ formulation of the second law of thermodynamics is satisfied for a relatively wide class of harmonic models. Even before the integration, the heat current has a positive definite spectrum because except for the difference $\vartheta_1 - \vartheta_2$, the integrand in (42) has a definite sign. This holds for any spectral densities $\rho_{1,2}$, be they “structured” (non-Markovian case) or flat. Our result differs strongly from the model of Ref. [8] that also considered two oscillators coupled to separate (local) baths and found for certain choices of parameters a violation of the second law. In that formulation, the heat current is proportional to

$$\dot{Q}_{1\rightarrow 2} \propto e^{\hbar \omega_{20}/T_2} - e^{\hbar \omega_{10}/T_1}$$

which is negative when $\omega_{10}/T_1 > \omega_{20}/T_2$ [the parameters taken in Fig. 3(right)]. The fact that the oscillator frequencies appear here outside any frequency integral may be traced back to the assumption that the coupling is based on the rotating-wave approximation (2) that preserves the total occupation number of the two oscillators. This is, however, a poor approximation when the eigenfrequencies differ significantly. The example presented here thus demonstrates that a non-equilibrium steady state consistent with thermodynamics can be constructed even with locally coupled baths. The anomalous behaviour in Ref. [8] is not likely due to the difference between local and global couplings (in the latter case, the baths couple to the normal modes of the coupled oscillators at their shifted eigenfrequencies), nor to the (non)Markovian character of the master equation (the present model is consistent whatever the memory of the friction kernels).

We may only speculate how an inverted heat current could appear in the present framework. A problem may arise from UV divergences when the momenta are coupled [see Eq. (2)] since that involves an additional factor $\omega^2$ compared to the coordinate coupling. One can also think of certain renormalisation schemes that operate a subtraction in the spectral densities $\rho_{1,2}(\omega)$, but then one should rather re-consider the physical meaning of the subtraction for the non-equilibrium problem. (The subtracted modes are a way to take into account a renormalised oscillator mass, for example.)
3.5 Fluctuation-dissipation relations

Before discussing the correlations in the non-equilibrium stationary state with respect to entanglement between the oscillators, we point out that in the case of equal bath temperatures, the correlation functions satisfy fluctuation-dissipation (FD) relations. This result is satisfying and perhaps not obvious because a canonical equilibrium state is imposed for the two heat baths alone, while the oscillators’ state is reached dynamically by solving the equations of motion. There are indeed system-bath models in the literature that have been criticized for yielding stationary states that do not conform with the canonical equilibrium state [32, 33, 5].

When the coupled oscillators are in a global equilibrium state with effective temperature \( \vartheta(\omega) \), the fluctuation–dissipation relation for the (complex) cross-correlation spectrum according to the convention (33) reads

\[
S_{ij}(\omega) = -2i \frac{\vartheta(\omega)}{\omega} \left[ R_{ji}(\omega) - R_{ij}^*(\omega) \right], \quad i, j = x, y
\]  
(44)

Here \( \vartheta(\omega) \) depends only on one temperature. The indices \( i, j \) enumerate the oscillator coordinates \( x, y \), and the set of linear response functions \( R_{ij} \) is defined by

\[
\langle x(\omega) \rangle = \sum_i R_{xi}(\omega) f_i(\omega)
\]  
(45)

They describe the response of the oscillator coordinate \( x \) to an external force acting on oscillator \( i \) (recall the absorption spectrum of Fig. 1) and are given for our model by the matrix elements in Eq. (22). Indeed, for this linear system, the same response function applies for an external force and for the Langevin forces themselves. The only difference is that for an external (classical) force, the average \( \langle x(\omega) \rangle \) is nonzero.

Proof of FD relation: The correlation spectrum is a special case of the general correlation (34). For \( A = x_i \) and \( B = x_j \), the response functions are \( \alpha_k = R_{ik} \) and \( \beta_l = R_{jl} \), so that (common argument \( \omega \) suppressed again)

\[
S_{ij} = \sum_k R_{ik}^* R_{jk} S_{Fk} = 4 \vartheta \sum_k R_{ik}^* R_{jk} \operatorname{Re}(\mu_k)
\]  
(46)

using Eqs.(19) with a common temperature in the last step. The response matrix \( R_{ij} \) of Eq. (22) is the inverse of \( K_{ij} \), the matrix in Eq. (20) that translates the equations of motion: \( R_{ik} K_{kl} = \delta_{il} \) (summation over double indices). Take the complex conjugate of this equation and multiply from the right with \( R_{jl}^* \):

\[
R_{ik}^* K_{kl}^* R_{jl} = R_{ji}
\]  
(47)

We subtract from this relation the expression one gets by multiplying \( R_{jl} K_{lk} = \delta_{jk} \) from the left with \( R_{ik}^* \), and get

\[
R_{ik}^* (K_{kl}^* - K_{lk}) R_{jl} = R_{ji} - R_{ij}^*
\]  
(48)
The matrix $K_{kl}$ on the left-hand side is symmetric [Eq. (20)] and its only elements with an imaginary part are the diagonal ones,

$$K_{kl}^* - K_{lk} = 2i\omega \text{Re}(\mu_k) \delta_{kl}$$

(49)

Inserting this into Eq. (48), we recognise the summand on the rhs of Eq. (46), and elementary algebra gives the fluctuation-dissipation relation (44) for the cross-correlation spectra $S_{ij}$. The FD relations of the baths is thus carried over to the oscillator pair, provided the system is globally in equilibrium.

Three remarks are in order. (1) The correlation functions involving momentum variables are easily dealt with using the equation of motion $\dot{x}_i = p_i/m_i$. This gives just a multiplicative factor in Fourier space. (2) The fluctuation–dissipation relation does not need a weak-coupling assumption and is valid for arbitrary $\lambda$ [3, 34]. In our case, both the fluctuation spectrum and the response functions have their poles shifted by the coupling between the oscillators, compared to the bare oscillators. (3) The Kubo–Martin–Schwinger (KMS) relations for correlation functions are also satisfied by the present model if the two bath temperatures coincide. They involve correlations with a fixed order of operators and state that their spectra satisfy $S_{AB}(\omega) = e^{-\hbar\omega/T}S_{BA}(\omega)$. This is obviously related to detailed balance. The KMS relations are used in the traditional proofs of the fluctuation–dissipation relations. Sometimes, however, they can be used to define thermal equilibrium in pathological cases where the canonical ensemble fails because its partition function diverges.

4 Entanglement

The concept of entanglement tries to identify and quantify correlations between the oscillators (or more generally between two parts of a system) that cannot be explained classically. Within the seminal discussion of Einstein, Podolsky and Rosen [21], such correlations suggest an incomplete, non-local, or non-realistic interpretation of the joint quantum state of two particles, adopting the language of Bell [35]. Entanglement measures have been developed over the last 20 years to quantify the amount of non-classical correlations, for example, using the magnitude of violating a Bell inequality. In the context of oscillators, entanglement theory speaks of continuous variables (rather than qubits or other finite-dimensional systems). See Ref. [36] for a review and original work by Duan et al. [37] and Simon [38]. Extensions to more than two oscillators were proven by Werner [39] and to non-Gaussian states in Refs. [40, 41, 42].

4.1 Covariances and optimal EPR correlations

The entanglement between the two oscillators in the stationary state may be characterised via their covariance matrix $C = (C_{ij})$ defined in Eq. (28), provided the state is Gaussian which is the case here [18]. This is a real symmetric $4 \times 4$-matrix that we write in the chosen basis $(q_i) = (x, p_x, y, p_y)$ in block form

$$C = \begin{pmatrix} A & C \\ C^T & B \end{pmatrix}$$

(50)
4.1 Covariances and optimal EPR correlations

The blocks $A$ and $B$ describe the covariances of oscillator $(x, p_x)$, resp. $(y, p_y)$, while the matrix $C$ describes correlations among the two oscillators. Its two-time version was given in Eq. (36). The Duan–Simon criterion [37, 38] states that the two oscillators are in a separable (i.e., non-entangled) state if and only if the following inequality is satisfied:

$$\det(A) \det(B) + \left|\det(C)\right| - \frac{1}{4} \hbar^2 \leq \frac{1}{4} \hbar^2 \left[\det(A) + \det(B)\right]$$

(We have adapted the formulation of Ref. [38] to dimensional positions and momenta.) Here, $I_4$ is the fourth invariant of the covariance matrix $C$ under local canonical transformations (the other three are the determinants in Eq. (51):

$$I_4 = \text{tr}(\sigma A \sigma C \sigma B \sigma C^T)$$

where $\sigma$ is the so-called symplectic matrix that collects the commutation relations among the phase-space coordinates

$$[q_i, q_j] = i\hbar \sigma_{ij}$$

In Eq. (52), a $2 \times 2$ version of $\sigma$ is used. A linear coordinate transformation $q_i \mapsto Q_i = \sum_j S_{ij} q_j$ on the total phase space is canonical if it preserves the commutation relations. Collecting $2 \times 2$ blocks into the symplectic matrix $\sigma$, this is equivalent to $S \sigma S^T = \sigma$. For details on linear canonical transformations and the symplectic groups $Sp(2), Sp(4)$ they form, see Refs. [43, 36, 44].

The physical meaning of the criterion (51) is that separable states never show Einstein-Podolsky-Rosen (EPR) correlations [37]. Recall that these correlations imply that for an entangled (gaussian) state, there is a pair $(Q, P)$ of sum or difference variables whose uncertainty product is below the Heisenberg limit, $\Delta Q \Delta P < \hbar/2$. This means that a measurement on one oscillator permits to infer the coordinates of the other one (‘EPR paradox’). In a symmetric situation, the EPR pair may be given by the combinations $Q = (x+y)/\sqrt{2}$ and $P = (p_x - p_y)/\sqrt{2}$. The point is not that such a situation would really violate the Heisenberg relation ($Q$ and $P$ actually commute in this example), but that for a separable state, the uncertainty product $\Delta Q \Delta P$ is bounded from below by $\hbar/2$, as shown in Ref. [37].

For the entanglement criterion of Refs. [37, 38], one diagonalises the so-called partially transposed covariance matrix

$$C^\Gamma = \Gamma C \Gamma$$

Here, the partial transposition acts as $\Gamma = \text{diag}(1, 1, 1, -1)$ in the basis $(x, p_x, y, p_y)$ [time reversal on oscillator $(y, p_y)$ alone]. The diagonalisation amounts to constructing a canonical coordinate transformation $S$ such that $S C^\Gamma S^T$ is diagonal. This procedure is called symplectic diagonalisation (see Appendix B). The smallest (symplectic) eigenvalue $\eta_{\text{min}}$ of $C^\Gamma$ provides the entanglement measure called logarithmic negativity [45, 44]

$$E_{12} = \log \frac{\hbar}{2\eta_{\text{min}}} \quad \text{if} \quad \eta_{\text{min}} < \hbar/2,$$

In the case $\eta_{\text{min}} \geq \hbar/2$, the two oscillators are separable ($E_{12} = 0$), although they may still be classically correlated. That can be quantified by the quantum mutual information or correlation entropy
4.1 Covariances and optimal EPR correlations

[44, 46]. This entropy considers the difference between the naive additive expectation for a composite system

\[ S_{12} = S_1 + S_2 - S_{\text{tot}} \]  \hspace{1cm} (56)

Here, entropies are computed according to von Neumann as \( S_{\text{tot}} = -\text{tr}(\rho_{12} \log \rho_{12}) \), while \( S_1 \) and \( S_2 \) are based on the reduced density matrices (tracing out the other oscillator). They coincide with the thermodynamic entropy in the thermal equilibrium state (canonical ensemble), up to a scale factor \( k_B \), but they are well-defined even out of thermal equilibrium. In the present example, \( \rho_{12} \) is the state of the two oscillators with the heat baths traced out. The sign \( S_{12} \geq 0 \) of the mutual information becomes plausible when we recall that \( S_1 \) and \( S_2 \) are computed from reduced states that are missing correlations between the systems. This is even true at the classical level. If the composite system is in an entangled pure state, then \( S_{\text{tot}} = 0 \) and the reduced states are mixed so that \( S_i > 0 \).

The symplectic eigenvalues and vectors of the covariance matrix come in pairs (Williamson theorem [47], Appendix B). We would like to point out that the eigenvectors corresponding to \( \eta_{\min} \) provide a simple way to construct an optimal EPR pair \((Q, P)\) of canonical coordinates

\[ Q = \sum_i (S \Gamma)_{1i} q_i, \quad P = \sum_i (S \Gamma)_{2i} q_i \]  \hspace{1cm} (57)

The matrix \( S \) is ordered such that the first two lines correspond to the eigenvalue \( \eta_{\min} \) of \( C^\Gamma \). The first two diagonal elements of \( S C^\Gamma S^T \) yield indeed

\[ \langle Q, Q \rangle_{12} = \eta_{\min} = \langle P, P \rangle_{12} \]  \hspace{1cm} (58)

while \( \langle Q, P \rangle_{12} = 0 \). Here, we have used the fact that the transformation \((Q, P) \mapsto (Q/r, rP)\) with \( r \neq 0 \) is canonical so that \( Q \) and \( P \) may be normalised to have the same physical dimension [homogeneous to \( \sqrt{\hbar} \) in this paper] and the same variance. Note that the averages in Eq. (58) are computed with respect to the non-equilibrium steady state. The only effect of the partial transposition \( \Gamma \) in Eq. (57) is that \( Q \) and \( P \) are no longer canonically conjugate: \([Q, P] \neq i\hbar\). This was already the case for the symmetric EPR pair introduced above. We conclude that since \( \langle Q, Q \rangle_{12} = \Delta Q^2 \), the two oscillators are EPR-correlated when \( \Delta Q \Delta P = \eta_{\min} < \hbar/2 \).

A comparison of the EPR correlations found in this way and the logarithmic negativity is shown in Fig. 4 where the “uncertainty product” \( \Delta Q \Delta P \) of the EPR pair is shown (curves with dots) for two parameter settings of Fig. 1, while increasing the coupling \( \lambda \). The data also show the mutual information (56). The crosses illustrate the so-called PPT criterion: the oscillators are PPT-entangled when the matrix \( C^\Gamma \) does not correspond to a physical state. (See Figure caption for more details.) The two criteria quantitatively agree on the onset of entanglement (the curves cross there). Our construction of the EPR pair has the advantage that it provides the experimenter with a definite measurement protocol: choose the generalised coordinates \( Q, P \) coming out of the symplectic eigenvectors and measure their correlations.

The results of Fig. 4 are for temperatures \( T_1, T_2 \ll \hbar \omega_1 \). We have evaluated the frequency integrals for the stationary covariance matrix elements numerically. Baths with a Drude cutoff for the spectral density are taken so that even the momentum correlations are UV-convergent. The diagonalisation of the covariance matrices \( C \) and \( C^\Gamma \) is done using the symplectic techniques of Appendix B. We present data for a non-equilibrium situation, but no qualitative changes appear when the two baths have similar temperatures.
4.1 Covariances and optimal EPR correlations

Covariances and optimal EPR correlations

Figure 4: (left) Covariances that test the entanglement between the two oscillators in the stationary state. Baths at low temperatures \( T_1 = 0.1 \hbar \omega_{10} \), \( T_2 = 0.15 \hbar \omega_{10} \). The curves marked (a, c) correspond to the parameters of Fig. 1, only the coupling between the oscillators is varied, expressed as \( g = (\lambda/m_1)^{1/2} \). The crosses visualise the PPT criterion for the partially transposed covariance matrix \( \Gamma^T \): when the smallest (ordinary) eigenvalue of the hermitean matrix \( \Gamma^T \) + \( i\hbar \sigma/2 \) falls below zero, the state is entangled [38]. (Our plot shifts this eigenvalue up by \( \hbar/2 \) so that entanglement appears below the same line.) The dots and curves give the uncertainty product \( \Delta Q \Delta P \) of the EPR coordinate combinations (58) in units of \( \hbar \), constructed from the smallest symplectic eigenvalue of \( \Gamma^T \). (right) Correlation entropy (mutual information) \( S_{12} \) [Eq. (56)] vs. the coupling.

One sees that low temperatures and large couplings lead to both correlations and entanglement. Off-resonant oscillators requires a larger coupling (to provide an efficient mixing in the normal modes). Entanglement appears when the chosen covariances are below the \( \hbar/2 \) threshold (horizontal line). Note that the mutual information \( S_{12} \) is not in a one-to-one correspondence with entanglement – this is related to the fact that the variances \( \Delta Q \Delta P \) (the eigenvalues \( \nu \) of the covariance matrix) are compared to the ‘quantum scale’ \( \hbar \) when dealing with entanglement. It is also remarkable that the EPR pair constructed above yields an ‘uncertainty product’ that falls, for entangled oscillators, even below the PPT criterion (marked by crosses). The two entanglement quantifiers coincide, in fact, for the special case that the two oscillators are in a so-called symmetric state (i.e., \( A \) and \( B \) have the same symplectic eigenvalues [44]), which is generally not the case here. In the plot, it is seen that the quantifiers coincide right at the entanglement threshold. This is proven analytically in Appendix B [after Eq. (83)].

The procedure of symplectic diagonalisation, although unfamiliar, also helps in evaluating the mutual information \( S_{12} \) of Eq. (56). The symplectic eigenvalues \( \nu_{\pm} \) of the covariance matrix \( \Gamma^T \) itself quantify, loosely speaking, the occupation of the normal modes \( \omega_{\pm} \). Indeed, they determine the von Neumann entropy of the Gaussian two-oscillator state as the simple sum [48] (Eq. (23) of Ref. [44])

\[
S_{\text{tot}} = f(2\nu_+/\hbar) + f(2\nu_-/\hbar)
\]

\[
f(x) = \frac{x + 1}{2} \log \frac{x + 1}{2} - \frac{x - 1}{2} \log \frac{x - 1}{2}
\]

Note that Eq. (60) only makes sense for \( \nu_{+, -} \geq \hbar/2 \): this is the criterion for a physical state. A partial entropy like \( S_1 \) in Eq. (56) is easily computed from the covariance matrix because the reduced states are determined by the block matrices \( A \) and \( B \). (Tracing out the other oscillator amounts to chopping off unobserved blocks of the covariance matrix.) For a single oscillator, the symplectic diagonalisation transforms \( A \) into a multiple of the unit matrix. We then get its symplectic eigenvalue...
\( \nu_A \) from the determinant \( \det A = \det (SAS^T) = \nu_A^2 \), and \( S_1 = f(2\nu_A/\hbar) \). (Linear canonical transformations have \( \det S = 1 \).)

### 4.2 Minimum noise quadratures in the frequency domain

We now combine the two methods of our analysis employed so far and introduce ways to quantify entanglement via frequency spectra that are available for the non-equilibrium state of the two oscillators (Sec. 3.3). The criteria for entanglement discussed so far provide an obvious motivation: the two oscillators are entangled when certain joint measurements (involving linear combinations of observables) show errors below the ground state uncertainties imposed by the Heisenberg relations. This suggests to analyse the spectrum \( S_{QQ} = \frac{1}{2} (S_{xx} + S_{yy} + 2S_{xy}) \) of the EPR variance \( Q = (x + y)/\sqrt{2} \) introduced above. But why prefer \( S_{PP} \) to \( S_{YY} \) with \( Y = (x - y)/\sqrt{2} \)? The two are related since, as noted above, the time derivative introduces just an additional factor \( \omega^2 \) into the spectrum. And what would be the “entanglement threshold” for such a spectrum?

The spectral representation of the correlation matrix \( C = (C_{ij}) \) gives us a matrix \( S_{ij}(\omega) \) that one may analyse for its local symplectic invariants. This is not of much use, however: from the block form for the spectrum of the off-diagonal sub-matrix \( C \) [see Eqs.(37, 50)], it is easy to check that at any frequency \( \omega \), this sub-determinant vanishes. The same is true for the spectra that give the sub-blocks A and B. Another quick calculation checks that the formula (52) for the fourth invariant, when applied to the sub-blocks of the spectral matrix \( S_{ij}(\omega) \), yields \( I_4 = 0 \), too. Whatever quantity should replace the term \( \hbar^2 \) in Eq. (52) in the spectral domain: the inequality (51) is satisfied as long as it is real.

To simplify the following discussion, it is convenient to scale the canonical coordinates \((x, p_x, y, p_y)\) in such a way that they have the same physical dimension. Recall that such a re-scaling was already used when we introduced the EPR pair \( Q \) and \( P \) with identical variances. The transformation in the \((x, p_x)\) plane we adopt is

\[
\begin{pmatrix} x \\ p \end{pmatrix} \mapsto \begin{pmatrix} \sqrt{k_1/\omega_{10}} \\ 0 \\ \frac{1}{\sqrt{m_1\omega_{10}}} \end{pmatrix} \begin{pmatrix} x \\ p \end{pmatrix}
\]

which is canonical if we set \( \omega_{10} = \sqrt{k_1/m_1} \). Note that we work here with the convention of re-scaling with the non-coupled eigenfrequencies. This is motivated by experimental approaches where two parties would have access to only one of the two oscillators, e.g., the parameters \( k_1, m_1 \) and the canonical pair \((x, p_x)\). Simple consequences are that for the time derivative, we now have \( \dot{x} = \omega_{10}p_x \), and the (bare) oscillator energy is \( H_1 = \omega_{10}(p^2 + x^2) \).

To search for spectral correlations, consider now a pair of coefficients \( \alpha_x, \alpha_p \) and form the linear combination \( a = \alpha_x x + \alpha_p p \). Switching to Fourier space, we have

\[
a(\omega) = \alpha_x x(\omega) - i(\omega/\omega_{10})\alpha_p x(\omega)
\]

The real coefficients thus combine in a natural way into a complex weight factor \( \alpha = \alpha_x + i(\omega/\omega_{10})\alpha_p \), as it happened when the general cross-correlation spectrum \( S_{AB} \) was introduced [Eq. (34)]. When computing the spectrum \( S_{aa} \), the global phase of \( \alpha \) drops out (because we focus on a stationary state).
This motivates to consider the following hermitean spectral matrix [taking $A, B = x, y$ in Eq. (34)]

$$S(\omega) = \begin{pmatrix} S_{xx}(\omega) & S_{xy}(\omega) \\ S_{yx}(\omega) & S_{yy}(\omega) \end{pmatrix}$$  \hspace{1cm} (63)$$

and to search for its (complex) eigenvectors in view of minimising covariance spectra. Indeed, a complex linear combination $q(\omega) = \alpha x(\omega) + \beta y(\omega)$ of the two oscillator coordinates would show a spectrum $S_{qq}(\omega) = (\alpha^*, \beta^*) S(\omega)(\alpha, \beta)^T$. This quadratic form can be minimised by choosing $(\alpha, \beta)$ as eigenvectors of $S$, that form the unitary matrix $U$ in the similarity transformation $S \mapsto U^\dagger S U = \text{diag}(S_{\text{min}}, S_{\text{max}})$.

We remark that such a construction can be understood in the time domain as a “linear filter” that maps the time series data $\{x(t), y(t)\}$ to

$$q(t) = \int d\tau \left\{ \alpha(\tau) x(t - \tau) + \beta(\tau) y(t - \tau) \right\}$$  \hspace{1cm} (64)$$

This convolution takes in Fourier space the simple form $q(\Omega) = \alpha(\Omega) x(\Omega) + \beta(\Omega) y(\Omega)$ and suggests certain constraints on the frequency-dependent coefficients $\alpha(\Omega)$ and $\beta(\Omega)$ (related to reality and causality). Such constraints may be relaxed, however, if one considers that the linear filter is applied to pre-recorded data measured by the experimenters who share their locally obtained data.

![Figure 5: Spectra of optimal covariance witnesses. (left) position variables, (right) momentum variables. Thin dashed lines: $T = 0$ limit for the variables $(x \pm y)/\sqrt{2}$ and $(p_x \pm p_y)/\sqrt{2}$. “EPR”: spectra for the fixed canonical coordinates $Q, P$ constructed in Sec. 4.1 that minimise the partially transposed covariance matrix. Magenta and orange: largest ($S_{\text{max}}$) and smallest ($S_{\text{min}}$) eigenvalue of the (hermitean) spectral matrix $S(\omega)$ [Eq. (63)]. Parameter set (b) of Fig. 1 in both panels, $T_1 = 0.5 \hbar \omega_{10} > T_2 = 0.25 \hbar \omega_{10}$.](image)

The result of this construction, per each frequency, is shown in the curves marked $S_{\text{max}}$ and $S_{\text{min}}$ in Fig. 5 where the largest (smallest) of the two eigenvalues is plotted. It is to be noted that the spectrum $S_{\text{min}}$ is close to or even below the lower of two “quantum limits” that we construct in the following way: consider the sum and difference quadratures $(x \pm y)/\sqrt{2}$ and compute their noise spectrum in the presence of all couplings, but at temperature $T = 0$ for both baths. These spectra show separate peaks at the normal mode frequencies. This is as expected, since in the lower (higher) normal mode the two oscillators move in phase (in phase opposition). It is remarkable that the EPR coordinates constructed from the “global” covariance matrix $C$ already achieve for certain frequencies a noise spectrum below this limit [red and blue curves in Fig. 5].
To conclude this discussion, we remark that the model presented here, being based on the assumption that the two baths are not correlated, may be considered as a kind of “separable reference” with respect to more general (non)classical correlations. It is well known that two systems that couple to the same bath experience stronger correlations since the polarisation of the bath translates into additional interactions (for example, the van der Waals interaction in atomic and molecular physics) \[49, 50, 51\]. The minimal correlation spectra can thus provide a reference: if arbitrary correlations between the Langevin forces are allowed for, one could imagine to get smaller covariance spectra (tighter EPR correlations). The presence of such correlations must be inferred when experimental data fall below the spectral minima constructed here. This may be expected in a situation of strong coupling when entanglement between the oscillators gets mapped via bath polarisation into the joint quantum state of the baths.

5 Conclusion

Coupled oscillators provide a paradigmatic example of system and bath models that can be analytically solved with the help of quantum Langevin equations, without any Markov approximations. In this paper, we have shown that a composite system whose parts are locally coupled to heat baths passes all thermodynamic consistency tests in the stationary state, be it non-equilibrium (different bath temperatures) or not. We have shown that the fluctuation–dissipation relations are satisfied for any choice of bath spectral density, provided the two bath temperatures coincide. If they differ, the heat current is found as a positive definite frequency integral in accordance with the Second Law. The anomalous heat current fromm cold to hot bath found in earlier work [8] is probably due to approximations applied in the modelling (rotating-wave approximation, Lindblad dissipation operators appropriate for resonant interactions). The criticism of the concept of locally coupled baths that arose in the wake of Ref. [8] does not seem justified in view of the results presented here.

The coupled oscillator model has the advantage that it can be applied flexibly to a plethora of physical systems. The mechanical oscillators in force microscopy and resonant electric circuits provide two typical examples where both weak and strong damping is relevant. The phonon bath in a solid can be easily modelled with a Debye spectral density that shows qualitatively different memory effects compared to the Ohm-Drude case used here in the numerical examples. One may even think of very different resonance frequencies as they appear in optomechanical systems (light from a laser cavity coupled to a mirror mounted on an oscillating membrane) \[52, 53, 54, 55, 56\], where the standard interaction (via radiation pressure) is mapped to a bilinear form under suitable approximations. Another hybrid system would be provided in atom chips \[57\] where the collective oscillation of an ultracold gas may be coupled to electronic resonances in a semiconducting microstructure. Finally, even electrons in a two-dimensional gas (or in a Penning trap) may be treated with the present formalism, the two position coordinates playing the role of the two oscillators. Magnetic fields then provide additional couplings that also involve mixed position-momentum terms, and different dampings may be engineered using anisotropic textures in the direct environment of the planar trap.

The spectral analysis of entanglement and correlations between the oscillator quadratures can
be developed further. We did not explore so far the constraints on the signal filter of Eq. (64) imposed by causality. The hermitean correlation spectrum having optimal eigenvectors whose global phase is arbitrary, there is some flexibility so that Kramers-Kronig relations may be not difficult to implement. An interesting perspective are spectral functions that characterise the broadening of a resonance due to friction. This concept may provide a expansion of the canonical commutator in the frequency domain based on the correlation $\langle [x(t), p_x(t')] \rangle$. By linear response theory, this is related to the absorption spectroscopy displayed in Fig. 1, and would clearly provide a quantum reference or threshold for correlations.

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A Derivation of the Langevin equations

A.1 Elimination of the bath variables

From the bath Hamiltonian (4) follows the equation of motion for the $j$th normal mode

$$\dot{p}_j + k_j q_j = k_j c_j x, \quad \dot{q}_j = p_j / m_j$$

(65)

Its solution with initial conditions $(q_j(0), p_j(0))$ is

$$q_j(t) = q_j(0) \cos \omega_j t + \frac{p_j(0)}{m_j \omega_j} \sin \omega_j t + \omega_j c_j \int_0^t dt' x(t') \sin \omega_j (t - t')$$

(66)

where $\omega_j = (k_j / m_j)^{1/2}$ is the normal mode frequency. The derivative of this expression gives the momentum $p_j(t)$. Since we are dealing with a linear system, both classical and quantum mechanics give the same result. The differences originate in the initial conditions.

Inserting this result into the equation of motion for the oscillator $(x, p_x)$, we get

$$\dot{p}_x + k_1 x = \lambda (y - x) - \delta k_1 x - \Gamma_1 [t, x] + \tilde{F}_1(t)$$

(67)

The coordinate $y$ corresponds to the other oscillator. The bath-induced shift in the spring constant $k_1$ is simply

$$\delta k_1 = \sum_{j \in B_1} k_j c_j^2$$

(68)

where $j \in B_1$ enumerates the set of bath modes. The frictional force is denoted by

$$\Gamma_1 [t, x] = - \int_0^t dt' x(t') \sum_{j \in B_1} k_j \omega_j c_j^2 \sin \omega_j (t - t')$$

(69)
and the Langevin force is the normal mode sum
\[ \tilde{F}_1(t) = \sum_{j \in B_1} c_j \left( k_j q_j(0) \cos \omega_j t + \omega_j p_j(0) \sin \omega_j t \right) \] (70)

A partial integration of Eq. (69) yields the equivalent form with a velocity-dependent friction
\[ \Gamma_1[t, x] = \int_0^t dt' \dot{x}(t') \sum_{j \in B_1} k_j c_j^2 \cos \omega_j (t - t') - \sum_{j \in B_1} k_j c_j^2 (x(t) - x(0) \cos \omega_j t) \] (71)

In the second line, the first term with \( x(t) \) cancels with the shifted spring constant \( \delta k_1 \) in Eq. (67). The second term with \( x(0) \) can be combined with the Langevin force \( \tilde{F}_1(t) \), leading to the replacement \( q_j(0) \mapsto q_j(0) - x(0) \) in Eq. (70). We denote in the following \( F_1(t) \) the Langevin force with these initial values.

To write the final form of the Langevin equation (11), we introduce the friction kernel
\[ \mu_1(t - t') = \Theta(t - t') \sum_{j \in B_1} k_j c_j^2 \cos \omega_j (t - t') \] (72)

A bath is by assumption a large system with a dense normal mode spectrum. Using the mode density \( \rho_1(\omega) \) of Eq. (5), one gets for the \( \mu_1(t - t') \) the integral representation (14) of the main text: it is the cosine transform of the bath spectral density \( \rho_1(\omega) \).

The correlation function of the Langevin force [see Eq. (70)] becomes with the averages of Eq. (8)
\[ \langle F(t), F(t') \rangle_T = \sum_{j \in B_1} c_j^2 \left\{ k_j \omega \langle (q_j(0) - x(0))^2 \rangle_T \cos \omega_j t \cos \omega_j t' + \omega_j^2 \langle p_j(0)^2 \rangle_T \sin \omega_j t \sin \omega_j t' \right\} \]
\[ = \sum_{j \in B_1} k_j c_j^2 \vartheta(\omega_j) \cos \omega_j (t - t') \] (73)

Using the definition of the bath spectral density from Eq. (5), this leads to the expression (17). Compute also the commutator
\[ [F(t), F(t')] = \sum_{j \in B_1} c_j^2 \{ k_j \omega \left[ q_j(0) - x(0), p_j(0) \right] \cos \omega_j t \sin \omega_j t' + \omega_j k_j \left[ p_j(0), q_j(0) - x(0) \right] \sin \omega_j t \cos \omega_j t' \} \] (74)

Note that the operator \( x(0) \) does not contribute. The other commutators combine into
\[ [F(t), F(t')] = i\hbar \sum_j c_j^2 k_j \vartheta \sin \omega_j (t' - t) \]
\[ = i\hbar \int_0^\infty \frac{d\omega}{\pi} \omega \rho(\omega) \sin \omega (t' - t) \] (75)
A.2 Ohmic friction with Drude regularisation

With the help of these expressions, one can show that the solution to the quantum Langevin equations is such that the operators \(x(t)\) and \(p_x(t)\) satisfy, at each time \(t \geq 0\) the canonical commutation relations. This appears because the frictional damping is compensated exactly by the (quantum) noise fed by the Langevin forces and provides another application of the fluctuation–dissipation theorem in its full quantum version.

A.2 Ohmic friction with Drude regularisation

As a simple example, consider a friction kernel in Drude form as follows

\[
\mu(\omega) = \frac{\gamma}{1 - i\omega\tau_c} \tag{76}
\]

It corresponds to a spectral density with a Lorentzian shape

\[
\rho(\omega) = \frac{\gamma/\tau_c^2}{\omega^2 + 1/\tau_c^2} \tag{77}
\]

The memory kernel is a simple damped exponential

\[
\mu(\tau) = \Theta(\tau) \frac{\gamma}{\tau_c} e^{-\tau/\tau_c} \tag{78}
\]

with a memory time \(\tau_c\). The Markov limit \(\tau_c \to 0\) provides a “skew” representation of the \(\delta(\tau)\) kernel with support in the domain \(\tau \geq 0\) only.

B Symplectic diagonalisation

The covariance matrix is the expectation value of the symmetrised correlations \(C_{ij} = \langle \hat{q}_i, \hat{q}_j \rangle_{12}\) where hats are used to distinguish canonical observables. The action of a linear canonical transformation \(S\) on this matrix is \(C = (C_{ij}) \mapsto SCST\). We choose the lines of \(S\) to provide the coefficients of normal coordinates as in Eq. (57), e.g., \(\tilde{Q} = \sum_i S_{1i}\hat{q}_i\). For simplicity, we write the coefficients (lines of \(S\)) in this linear combination just \(\tilde{Q}^T = (S_{1i}), P^T = (S_{2i}), \ldots\) (without the hat). This leads to the simple notation \(\Delta \tilde{Q}^2 = \langle \tilde{Q}, \tilde{Q} \rangle_{12} = Q^T C Q\).

The symplectic diagonalisation is constructed via the (non-hermitean) eigenvalue problem

\[
-i\sigma C v = \eta v \tag{79}
\]

where \(\sigma\) is the \(4 \times 4\) symplectic matrix defined in Eq. (53). The right eigenvector \(v\) encodes in its real and imaginary parts the coefficients for the new position and momentum coordinates: \(v = Q + iP\). (We assume \(\eta > 0\), otherwise take the complex conjugate and work with \(v = Q - iP\). The arbitrary phase of \(v\) can be exploited to choose \(Q\) such that its overlap with the displacement coordinates \(x\) and \(y\) is maximal.) Multiply from the left with \(-i(Q^T - iP^T)\sigma\) and get \((\sigma^2 = -1)\)

\[
(Q^T - iP^T)C(Q + iP) = -i\eta(Q^T - iP^T)\sigma(Q + iP) \tag{80}
\]

The imaginary part of this yields

\[
Q^T C P - P^T C Q = -\eta(Q^T \sigma Q + P^T \sigma P) \tag{81}
\]
both sides are zero: on the left because $C$ is symmetric, on the right because $\sigma$ is anti-symmetric. Taking the real part:

$$Q^T C Q + P^T C P = 2\eta Q^T \sigma P$$  \hspace{1cm} (82)$$

We normalise the canonical coordinates such that $Q^T \sigma P = 1$, ensuring that for the corresponding operators, $[\hat{Q}, \hat{P}] = i\hbar$. Repeating this construction for all positive eigenvalues of $-i\sigma C$, the transformation matrix is built from the $Q$’s and $P$’s as line vectors; it satisfies $S\sigma S^T = \sigma$.

Multiplying Eq. (79) with $-i(Q^T + iP^T)\sigma$ from the left, the same reasoning yields the additional information that $Q^T C P = 0$ (the coordinates $\hat{Q}$, $\hat{P}$ are not correlated) and that the variances $\Delta \hat{Q}^2 = Q^T C Q$ and $P^T C P$ are equal. Therefore, from Eq. (82) the uncertainty product is $\Delta \hat{Q}\Delta \hat{P} = \eta$.

For the moment, we dealt with finding the normal modes of the covariance matrix $C$ itself. For the construction of an EPR pair $\hat{Q}$, $\hat{P}$ that detects entanglement between the two oscillators, we perform the above construction with the partially transposed covariance matrix $C^\Gamma = \Gamma C \Gamma$ [Eq. (54)]. Be $u'$ thus the eigenvector of $-i\sigma C^\Gamma$ with the smallest positive eigenvalue $\eta$. We decompose it $Q'+iP' = u'$ and normalise the $Q'$, $P'$ as before. Setting then $Q = \Gamma Q'$ and $P = \Gamma P'$, we get a pair whose variances with respect to $C$ are given by $\Delta \hat{Q} = \Delta \hat{P} = \sqrt{\eta}$. They are not necessarily canonically conjugate, but this is actually required to have sub-classical correlations $\eta < \hbar/2$.

In contrast to the above procedure, the PPT criterion performs a positivity check of the partially transposed state [38]. This can be done by looking for the eigenvalues of the hermitean matrix $C^\Gamma + \frac{1}{2}\sigma$. This eigenvalue problem

$$\left(C^\Gamma + \frac{1}{2}\sigma\right)u = \varepsilon u$$  \hspace{1cm} (83)$$

or

$$-i\sigma C^\Gamma u = -\frac{1}{2}u - i\varepsilon u$$

typically involves complex eigenvectors $u$. They yield complex coefficients for a linear combination of the canonical coordinates, $\hat{a} = \sum_i u_i \hat{q}_i$, like the familiar raising and lowering operators.

In the special case $\vareferencees

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