Quantum Thermal Conductivity and Brownian Motion in a Harmonic Chain

state of my diploma thesis

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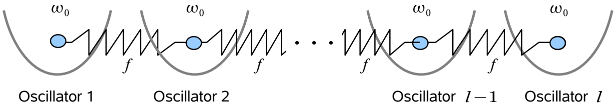
Outline

Introduction

- We want to understand the mechanism of heat conduction microscopically.
- Classical calculations have shown that harmonic chains exhibit anormal heat conduction: The heat flux is independent of the length of the chain.
- There is evidence for anormal heat conduction in carbon nanotubes.
- Are there new features in the quantum mechanical regime?

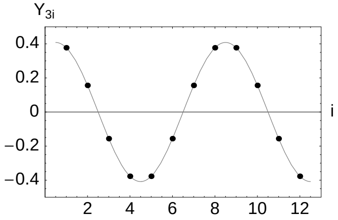
The Model
The chain

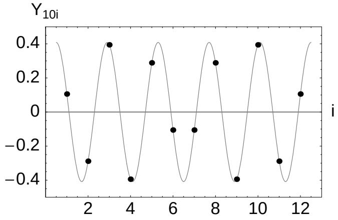


A chain consisting of l coupled harmonic oscillators with unity mass and frequency ω_0

$$H_c = \sum_{n=1}^{l} \left(\frac{1}{2} P_n^2 + \frac{1}{2} \omega_0^2 X_n^2 \right) + \sum_{n=1}^{l-1} \frac{f}{2} (X_{n+1} - X_n)^2$$

The Modes of the Harmonic Chain



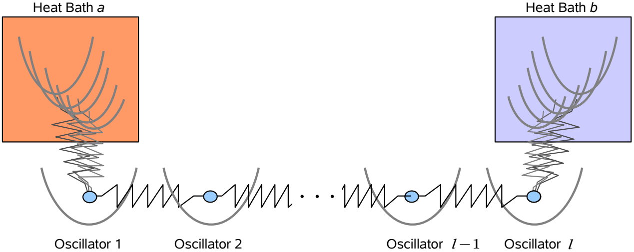


Some modes of a harmonic chain

- The normal modes are denoted as Y_i,
  the corresponding momenta are denoted as Q_i.
- Dispersion relation: $\omega^2 - \omega_0^2 = 4f \sin^2\left(\frac{k_i}{2}\right)$, $\qquad k_i = \pi \frac{i}{l}$
- The amplitude at the chain ends decreaes with frequency.
- Transformation matrix: $Y_n = \sum_{i=1}^{l} \left(G^t\right)_{ni} X_i$

The Model

The heat baths



Two identical heat baths at different temperatures T_a and T_b are coupled to the first and to the last oscillator of the chain:

$$H_{B\alpha} = \sum_{i=1}^{N} \left[\frac{p_{\alpha i}^2}{2} + \frac{1}{2}\omega_i^2 \left(x_{\alpha i} - \frac{c_i}{\omega_i^2} X_\beta \right)^2 \right], \quad (\alpha, \beta) \in \{(a,1),(b,l)\}$$

Heisenberg Equations of Motion

We use the Hamiltonian $H = H_c + H_{Ba} + H_{Bb}$ to set up the Heisenberg equations of motion:

$$\frac{dX_n}{dt} = \frac{i}{\hbar}[H, X_n] = P_n$$
$$\ddot{X}_n(t) = -\left(\omega_0^2 + 2f\right) X_n(t) + f\left(X_{n-1} + X_{n+1}\right) \qquad \text{für } 1 < n < l$$

The first and the last oscillator are affected by the baths:

$$\ddot{X}_1(t) = \dot{P}_1 = \frac{i}{\hbar}[H, P_1]$$
$$= -\left(\omega_0^2 + f + \sum_{i=1}^{N} \frac{c_i^2}{\omega_i^2}\right) X_1(t) + \sum_{i=1}^{N} c_i x_{1i}(t) + f X_2(t)$$

The equation for X_l is analog.

Eliminating the Baths' Degrees of Freedom

The Langevin Equations

- Solve the equations of motion for the bath degrees of freedom

$$\ddot{x}_{ai}(t) = -\omega_i^2 x_{ai}(t) + c_i X_1(t)$$

as a function of $X_1(t)$:

$$x_{ai}(t, X_1(t)) = f(x_{ai}(0), p_{ai}(0), t) + \frac{c_i}{\omega_i} \int_0^t dt' \sin\left(\omega_i(t - t')\right) X_1(t')$$

- Substituting $x_{ai}(t, X_1(t))$ into the equation of motion for X_1 one can summarize the influence of the bath as a noise function $\eta_a(t)$ and a damping function $\gamma(t')$:

$$\ddot{X}_1(t) = -\left(\omega_0^2 + f\right) X_1(t) + f X_2(t) - \gamma(t) X_1(0) - \int_0^t dt' \gamma(t - t') \dot{X}_1(t') + \eta_a(t)$$

$$\ddot{X}_2(t) = -(\omega_0^2 + 2f) X_2 + f X_1 + f X_3, \ \ldots \qquad \text{(Langevin equations)}$$

The Noise Function

- The initial conditions of the baths enter into the noise term.
- The noise has zero time average

$$\langle \eta_a(t) \rangle = \langle \eta_b(t) \rangle = 0$$

- In the limit of infinite heat baths the symmetrical autocorrelation function reads

$$\begin{aligned} K_k(t-t') &= \frac{1}{2}\left(\langle \eta_k(t)\eta_k(t')\rangle + \langle \eta_k(t')\eta_k(t)\rangle\right) \qquad k \in \{a, b\} \\ &= \frac{1}{\pi}\int_0^\infty d\omega \gamma \hbar\omega \frac{\Gamma^2}{\Gamma^2+\omega^2} \coth\left(\frac{1}{2}\frac{\hbar\omega}{k_B T_k}\right)\cos(\omega(t-t')) \end{aligned}$$

  with the cutoff Γ
- $K_k(t-t')$ is not a δ-function $\Rightarrow$ no white noise

The Damping Function

$$-\gamma(t)X_1(0) - \int_0^t dt'\gamma(t-t')\dot{X}_1(t')$$

- In the limit of infinite heat baths the damping function reduces to

$$\gamma(t) = \gamma\Gamma e^{-\Gamma|t|}$$

- Only in the limit of $\Gamma \to \infty$ this reduces to a δ-function which means Ohmic damping.

Solving the Langevin equations

$$\ddot{X}_1(t) = -\left(\omega_0^2 + f\right) X_1(t) + fX_2(t) \\ - \gamma(t)X_1(0) - \int_0^t dt' \gamma(t-t')\dot{X}_1(t') + \eta_a(t)$$

$$\ddot{X}_2(t) = -(\omega_0^2 + 2f)X_2 + fX_1 + fX_3, \ \ldots \qquad \text{(Langevin equations)}$$

- Transform to the normal coordinates of the pure chain to ge rid of the coupling f
- Go to Laplace space:
  - The convolution transforms to a product $s\hat{\gamma}(s)\hat{X}_1(s)$.
  - The differential equation becomes an algebraic equation.

Solving the Langevin equations

For each mode one gets the equation

$$\overbrace{\left[(s^2+\Omega_j^2)\delta_{ij} + s\hat{\gamma}(s)\left(G_{1i}G_{1j}+G_{li}G_{lj}\right)\right]}^{=:\hat{B}_{ij}(s)}\hat{Y}_j(s) = \left[G_{1i}\hat{\eta}_a(s)+G_{li}\hat{\eta}_b(s)\right] + sY_i(0) + Q_i(0)$$

With $\hat{A}(s) = \hat{B}(s)^{-1}$ one finds

$$\hat{Y}_j(s) = \sum_k s\hat{A}_{jk}(s)Y_k(0) + \sum_k \hat{A}_{jk}(s)Q_k(0) + \hat{F}_j^a(s)\hat{\eta}_a(s) + \hat{F}_j^b(s)\hat{\eta}_b(s)$$

$$F_j^a(s) = \sum_k G_{1k}\hat{A}_{jk}(t) \qquad F_j^b(s) = \sum_k G_{lk}\hat{A}_{jk}(t)$$

The Solution of the Langevin Equations

The inverse Laplace transformation yields

$$Y_j(t) = \sum_{k=1}^{l} \left[\dot{A}_{jk}(t) Y_k(0) + A_{jk}(t) Q_k(0) \right] + \int_0^t dt' \left[F_j^a(t-t') \eta_a(t') + F_j^b(t-t') \eta_b(t') \right]$$

With the response functions $F_j(t)$ for the noise
and the response functions $A_{jk}(t)$ for the initial conditions of the chain.

- In the limit of infinite baths all response functions decay exponentially with time.
- In the stationary case only the noise integrals are relevant.

The Noise Response Functions

The noise response function for one of the even normal mode reads

$$F_j^a(t) = \sum_{k=0}^{l_e} f_{jk}^a e^{\lambda_k^e t} + c.c. \qquad \text{with } l_e = \# \text{ even normal coordinates}$$

$$\approx f_{jj}^a e^{\lambda_j^e t} + c.c. \qquad \lambda_j^e \approx -\epsilon_r + i\,\Omega_j$$

- $\mathrm{Re}(\lambda_i^e) < 0$, i.e. $F_j^a(t)$ decays exponentially.
- There is no mixing between even and odd normal coordinates.

Calculating the Symmetrical Correlations

Due to the uncertainty principle we cannot calculate trajectories but only expectation values.

$$\langle X_i \rangle = \langle Y_i \rangle = \langle P_i \rangle = \langle Q_i \rangle = 0$$

We are interested in the correlations!

We use the solution of the Langevin equations

$$Y_j(t) = \sum_{k=1}^{l} \left[\dot{A}_{jk}(t) Y_k(0) + A_{jk}(t) Q_k(0) \right] + \int_0^t dt' \left[F_j^a(t-t')\eta_a(t') + F_j^b(t-t')\eta_b(t') \right]$$

to calculate e.g. the symmetrical correlation $\frac{1}{2} \langle \{ Y_i(t), Y_j(t) \} \rangle$

The Stationary Correlations

For the stationary correlations we only consider the noise integrals

$$\frac{1}{2}\langle\{Y_i(t),Y_j(t)\}\rangle = \int_0^t dt' \int_0^t dt'' \Big[F^a_{Y_i}(t-t')F^a_{Y_j}(t-t'')K_a(t'-t'') + F^b_{Y_i}(t-t')F^b_{Y_j}(t-t'')K_b(t'-t'')\Big]$$

$$F^a_j(t) = \sum_{k=0}^{l_e} f^a_{jk} e^{\lambda^e_k t} + c.c.$$

$$K_k(t-t') = \frac{1}{2}\big(\langle\eta_k(t)\eta_k(t')\rangle + \langle\eta_k(t')\eta_k(t)\rangle\big) \qquad k\in\{a,b\}$$
$$= \frac{1}{\pi}\int_0^\infty d\omega\gamma\hbar\omega\frac{\Gamma^2}{\Gamma^2+\omega^2}\coth\left(\frac{1}{2}\frac{\hbar\omega}{k_B T_k}\right)\cos(\omega(t-t'))$$

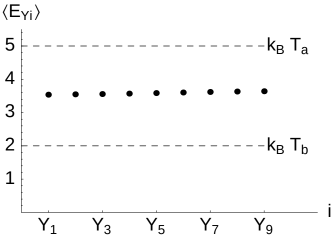
Evaluating $\frac{1}{2}\langle\{Y_i(t), Y_j(t+\tau)\}\rangle$

- Exchange the double sum and the integrations
- Exchange time integration and ω-integration

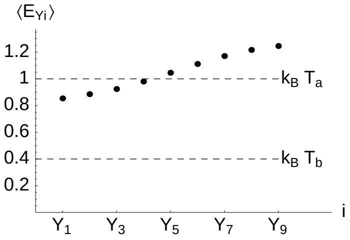
$$\int dt' \int dt'' \int d\omega \sum_{k,k'} f(t', t'', \omega, \lambda_k, \lambda_{k'})$$
$$= \sum_{k,k'} \int d\omega \int dt' \int dt'' f(t', t'', \omega, \lambda_k, \lambda_{k'})$$

- Time integrals can be solved analytically
- Compute ω-integral numerically

Results: Energy in Normal Modes



(a) $k_B T_a = 5,\ k_B T_b = 2$



(b) $k_B T_a = 1,\ k_B T_b = 0.4$

Figure: Energy in the normal modes

- High temperature regime: $\langle E_{Yi} \rangle \approx k_B \frac{1}{2}(T_a + T_b)$
- Low Temperature regime: Zero point energy $\Rightarrow \langle E_{Yi} \rangle \approx \hbar\Omega_i/2$

Occupation Numbers $n_i = \frac{E_{Yi}}{\hbar\Omega_i} - \frac{1}{2}$

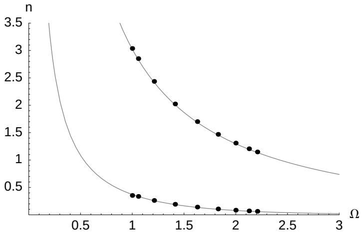


Figure: Occupation numbers for the normal modes, upper curve: $k_B T_a = 5$, $k_B T_b = 2$, lower curve $k_B T_a = 1$, $k_B T_b = 0.4$

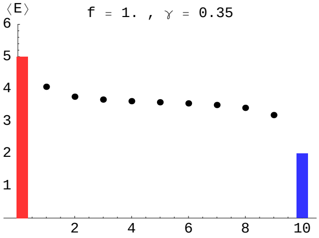
- Good agreement with Bose-Einstein distribution $n_i = \frac{1}{\exp\left(\frac{\hbar\Omega_i}{k_B T}\right) - 1}$

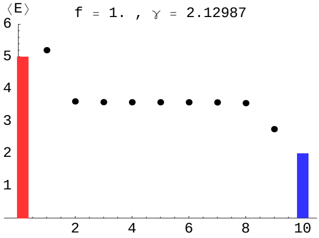
  i.e. normal modes have a common temperature

Temperature Profiles

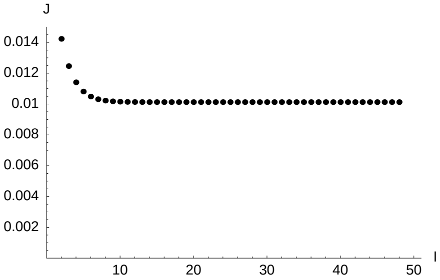
- Transform the correlations back to real space coordinates
- We use the average local energy $\langle E_i \rangle$ as a measure for the temperature

$$\langle E_i \rangle = \frac{1}{2}(\omega_0^2 + 2f)\left\langle X_i^2 \right\rangle - \frac{1}{2} f\left(\langle X_i X_{i+1} \rangle + \langle X_i X_{i-1} \rangle\right) + \frac{1}{2}\left\langle P_i^2 \right\rangle$$





Heat Current and the Length of the Chain

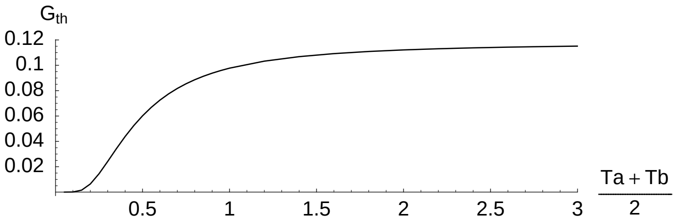


Stationary energy current for different chain lengths l
Parameter: $\gamma = 0.35$, $f = 1$, $k_B T_a = 0.5$, $k_B T_b = 0.2$, $\Gamma = 10$

- The energy current is independent of the length of the chain.
  $\Rightarrow$ anormal heat conduction
- Anormal heat conduction also in the quantum mechanical regime

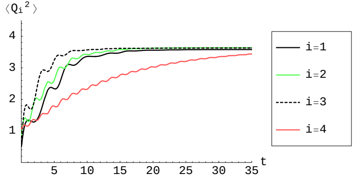
Thermal Conductivity as a Function of Temperature

$$G_{th} = \frac{J}{T_a - T_b}$$

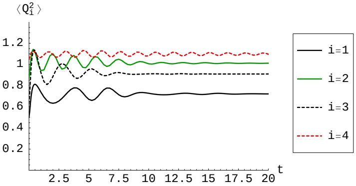


- In the classical regime $k_b T \gg \hbar\Omega_i$ the thermal conductivity is constant.
- In the low temperature regime the thermal conductivity behaves like the occupation number $\propto e^{-\frac{k_B T}{\hbar\Omega}}$

Time Evolution



High temperature regime, $k_B T_a = 5, k_B T_b = 2$



Low temperature regime, $k_B T_a = 0.5, k_B T_b = 0.2$

Entanglement: Logarithmic Negativity

Correlations between coordinates and momenta

$\downarrow$

Logarithmic Negativity

[e.g: M. B. Plenio, J. Hartley, J. Eisert, New J. Phys. **6**, 36 (2004)]

Calculating the Logarithmic Negativity

- Create the $2l \times 2l$-Matrix

$$S = 2 \left(\begin{array}{c|c} \langle X_i X_j \rangle & \langle X_i P_j \rangle \\ \hline \langle P_i X_j \rangle & \langle P_i P_j \rangle \end{array} \right)$$

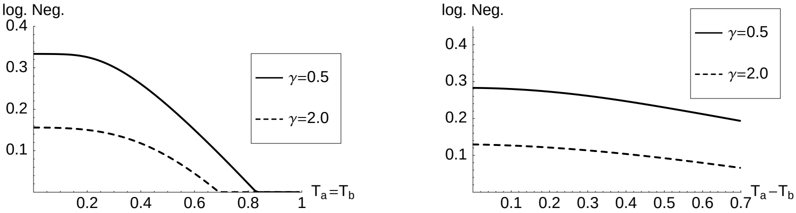
- Divide the system into two subsystems A and B
- Invert the momenta in one subsystem: $S \to S^T$
- Calculate the symplectic Eigenvalues of S^T, i.e. the sqareroot of the Eigenvalues of

$$-\sigma S^T \sigma S^T \qquad \text{with} \quad \sigma = \begin{pmatrix} 0 & \mathbb{I} \\ -\mathbb{I} & 0 \end{pmatrix}$$

- The logarithmic negativity is then given as

$$N = - \sum_{\substack{j=1 \\ |s_j|<1}}^{l} \log_2 (|s_j|)$$

Entanglement and Temperature

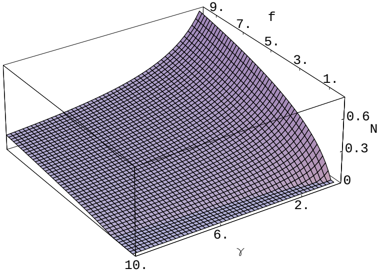


$T_a = T_b$ $\qquad$ $k_B T_a + k_B T_b = 0.7$

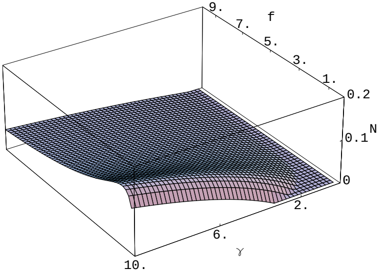
Figure: Original coordinates: $A = \{X_1\}, B = \{X_2, X_3\}$, $f = 2$

- Entanglement breaks down with temperature.
- Entanglement decreases slightly with temperature difference.

Entanglement and the Couplings f and γ



Original coordinates:
$A = \{X_1\}, B = \{X_2, X_3\}$



Normal coordinates:
$A = \{Y_1\}, B = \{Y_2, Y_3\}$

$$k_B T_a = 0.5,\ k_B T_b = 0.2$$

- f favors entanglement between the original coordinates.
- γ favors entanglement between the normal modes.

Time Evolution of Entanglement

Example: $l = 4,\ f = 1,\ \gamma = 0.5,\ k_B T_a = 0.5,\ k_B T_b = 0.2$

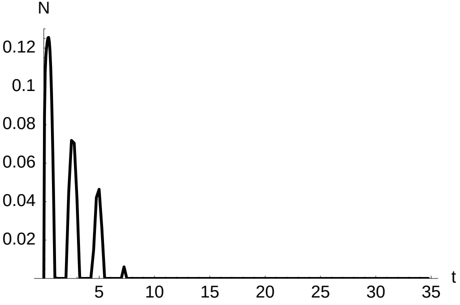


Figure: Entanglement within the normal coordinates of the chain, $A = \{Y_1\}, B = \{Y_2, Y_3, Y_4\}$

- No initial and no stationary entanglement but **temporary entanglement**
- There is never entanglement between even and odd modes.

Disorder

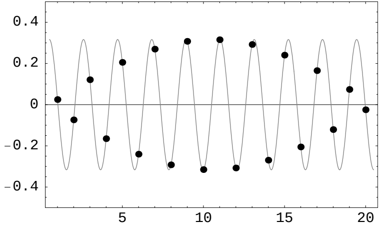
Motivation

- From classical considerations it is known that harmonic chains show diverging heat conductivity, because anharmonicities are necessary for diffusion due to Umklapp-Processes. An alternative which conserves the linearity of the system is the introduction of disorder.

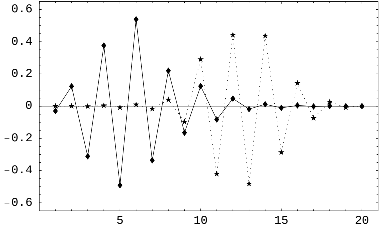
Changes to the ordered chain

- We choose either the onsite potentials randomly: $\omega_0 \longrightarrow \omega_i$ or the coupling constants: $f \longrightarrow f_i$
- The inversion symmetry of the system breaks down.
- Anderson localisation occurs.

Localisation of the Normal Modes



(a) Ordered chain



(b) Disorder: $f_i = 1 \pm 0.2$

Figure: The highest normal modes (Disorder: Two typical realizations)

- Normal modes have lower amplitudes at the ends of the chain
- Normal modes have different amplitudes at left and right end of the chain
  $\Rightarrow$ Strong coupling to one bath, weak coupling to the other bath

Occupation Numbers

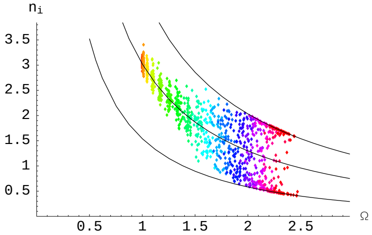
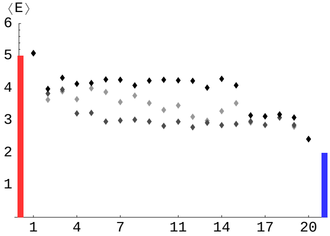


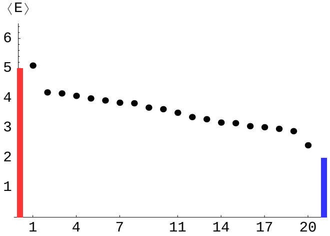
Figure: Occupation numbers of a disordered chain, 50 realizations. $l = 20,\ \gamma = 2,\ k_B T_a = 5,\ k_B T_b = 2$

- Modes with high frequency are strongly localized
- Localized modes are coupled more strongly to one bath than to the other.
- Low frequency modes are coupled more or less equally to both baths.

Temperature Profiles



(a) Some single realizations

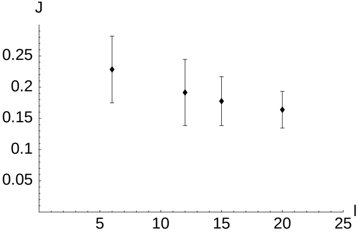


(b) Average over 50 realizations

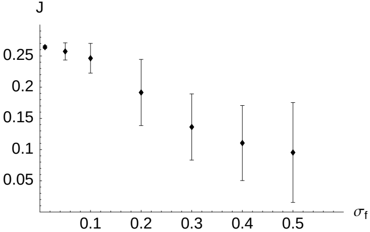
$$f_i = 1 \pm 0.2,\ k_B T_a = 5,\ k_B T_b = 2$$

Temperature Profiles

The mean heat current



as a function of the chain length l ($f_i = 1 \pm 0.2$)



as a function of the standarddeviation of σ_f ($l = 12$)

Looks like normal heat conduction (like the classical case).

Conclusions

- Like in classical systems the heat conduction is anormal in the ordered quantum mechanical case.
- We see several new faetures in the quantum mechanical regime:
  - The heat conductivity breaks down in the low temperature regime.
  - One can observe entangelement inside the chain.
  - Energies are dominated by zero point energies
- In the disordered case we find normal heat conduction like in the classical case. Further investigations are to be done about the low temperature disordered case.

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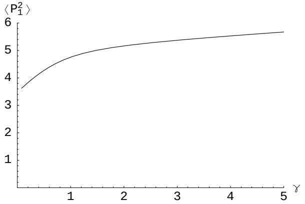
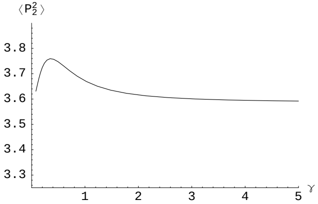
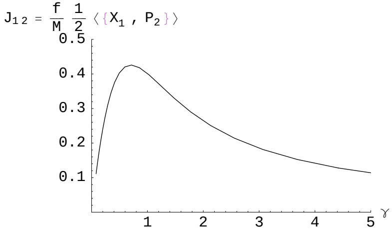
Dependence on the Coupling to the Baths γ





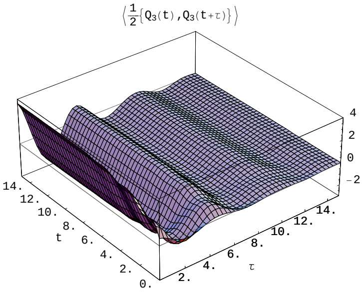


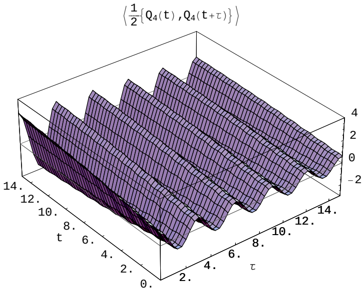
$f = 1$

Energy current
and some local temperatures

- The thermal contact between boundary oscillators and the rest of the chain breaks down when γ gets too big.

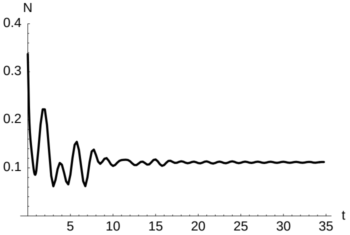
Time Shifted Correlations



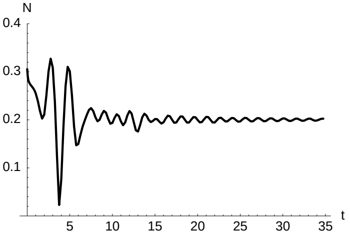


Time of Entanglement (Original Coordinates)

Example: $l = 4$, $f = 1$, $\gamma = 0.5$, $k_B T_a = 0.5$, $k_B T_b = 0.2$



(a) $A = \{X_1\}, B = \{X_2, X_3, X_4\}$



(b) $A = \{X_1, X_2\}, B = \{X_3, X_4\}$

Figure: Entanglement within the oscillators of the chain