

**Zeitschrift:** Helvetica Physica Acta  
**Band:** 62 (1989)  
**Heft:** 6-7

**Artikel:** Quantum mechanical harmonic chain attached to heat baths  
**Autor:** Zürcher, U. / Talkner, P.  
**DOI:** <https://doi.org/10.5169/seals-116168>

#### Nutzungsbedingungen

Die ETH-Bibliothek ist die Anbieterin der digitalisierten Zeitschriften auf E-Periodica. Sie besitzt keine Urheberrechte an den Zeitschriften und ist nicht verantwortlich für deren Inhalte. Die Rechte liegen in der Regel bei den Herausgebern beziehungsweise den externen Rechteinhabern. Das Veröffentlichen von Bildern in Print- und Online-Publikationen sowie auf Social Media-Kanälen oder Webseiten ist nur mit vorheriger Genehmigung der Rechteinhaber erlaubt. [Mehr erfahren](#)

#### Conditions d'utilisation

L'ETH Library est le fournisseur des revues numérisées. Elle ne détient aucun droit d'auteur sur les revues et n'est pas responsable de leur contenu. En règle générale, les droits sont détenus par les éditeurs ou les détenteurs de droits externes. La reproduction d'images dans des publications imprimées ou en ligne ainsi que sur des canaux de médias sociaux ou des sites web n'est autorisée qu'avec l'accord préalable des détenteurs des droits. [En savoir plus](#)

#### Terms of use

The ETH Library is the provider of the digitised journals. It does not own any copyrights to the journals and is not responsible for their content. The rights usually lie with the publishers or the external rights holders. Publishing images in print and online publications, as well as on social media channels or websites, is only permitted with the prior consent of the rights holders. [Find out more](#)

**Download PDF:** 08.08.2025

**ETH-Bibliothek Zürich, E-Periodica, <https://www.e-periodica.ch>**

## Quantum Mechanical Harmonic Chain Attached to Heat Baths

U. Zürcher, P. Talkner, Institut f. Physik, Universität Basel  
Klingelbergstr. 82, CH-4056 Basel

### Abstract

We study nonequilibrium properties of a quantum mechanical harmonic chain in the stationary state.

### 1. Outline of the model

We investigate a finite linear chain of  $N$  equal particles connected by equal harmonic springs, whose left and right ends are in contact with independent stochastic heat baths at temperatures  $T_1$  and  $T_N$ . These heat baths induce both fluctuations and dissipation in the chain. In its classical version this model has been studied in [1]. In [2] it was shown that a system of coupled oscillators can be made a model of a heat bath. Our starting point are the corresponding quantum Langevin equations for the operators  $x_n, p_n$  of the displacement of the  $n$ -th particle out of its equilibrium position and its conjugate momentum, respectively,

$$\frac{d}{dt}x_n(t) = p_n(t), \quad (1)$$

$$\begin{aligned} \frac{d}{dt}p_n(t) = & -2x_n(t) + x_{n+1}(t) + x_{n-1}(t) \\ & -\gamma(\delta_{1n} + \delta_{Nn})p_n(t) + \delta_{1n}E_1(t) + \delta_{Nn}E_N(t) \end{aligned} \quad (2)$$

subject to the boundary condition  $x_0(t) = 0, x_{N+1}(t) = 0$ . Here,  $\gamma$  denotes the damping constant,  $E_i(t), i = 1, N$  are the random force operators and  $\delta_{ij}$  is the Kronecker  $\delta$ . In Eqs. (1), (2) we have introduced scaled operators and constants by measuring time in units of the invers of the half Debye frequency. The Gaussian random force operators  $E_i(t)$  have vanishing mean,  $\langle E_i(t) \rangle = 0$ , and their second moments are determined by the commutator

$$[E_i(t), E_j(s)] = \delta_{ij}2i\hbar\gamma\frac{\partial}{\partial t}\delta(t-s), \quad (3)$$

and the symmetrized mean

$$\frac{1}{2} \langle E_i(t)E_j(s) + E_j(s)E_i(t) \rangle = \delta_{ij} \frac{\gamma}{\pi} \int_0^\infty d\omega \hbar\omega \coth\left(\frac{\hbar\omega}{2k_B T_i}\right) \cos\omega(t-s). \quad (4)$$

Here, the average  $\langle \rangle$  is taken with respect to the quantum mechanical canonical ensemble of the heat baths. Note that in the classical limit  $E_i(t)$  becomes a white random force. From Eqs. (1), (2) we derive the equations of motion for the equal time correlation functions for the operators  $x_n, p_n$ , i.e.  $\langle x_n(t)x_m(t) \rangle, \langle x_n(t)p_m(t) \rangle$ , etc. With the use of the fact that for linear systems the response function is equal in classical and quantum mechanics, we are able to determine the full covariance matrix explicitly.

## 2. Results

We have studied in some detail the stationary properties of the covariance matrix in the limit  $N \rightarrow \infty$ . The stationary heat flux through the chain is proportional to the work done on the  $i$ -th particle by its left neighbour, i.e.  $j \propto \langle x_{i-1}p_i \rangle$ . We find

$$j = \frac{e^{-\delta}}{\gamma} [\tilde{j}(T_1, \gamma) - \tilde{j}(T_N, \gamma)], \quad (5)$$

where the quantity  $\delta$  is defined by  $\gamma^{-1} = 2 \sinh(\frac{\delta}{2})$ . This leads to an infinite thermal conductivity. In the classical limit we recover  $\tilde{j}(T, \gamma) = T$ . In the quantum region, i.e. temperatures much below the Debye temperature of the chain,  $\Theta_D$ , we find

$$\tilde{j}(T, \gamma) \simeq \hbar r(\gamma) + \hbar s(\gamma) \left(\frac{T}{\Theta_D}\right)^4, \quad (6)$$

where  $r(\gamma)$  and  $s(\gamma)$  are smoothly varying functions of the damping constant. It is an interesting quantum phenomenon that the heat flux is strongly suppressed when both heat baths are at very low temperatures. This and the temperature profile along the chain shall be discussed elsewhere [3].

## 3. References

- [1] Z. Rieder, J. L. Lebowitz, and E. H. Lieb, J. Math. Phys. 8, 1073 (1967)
- [2] G. W. Ford, M. Kac, and P. Mazur, J. Math. Phys. 6, 504 (1965)
- [3] U. Zürcher, P. Talkner, to be published