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Quantum Mechanical Harmonic Chain Attached to Heat Baths

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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,

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

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

subject to the boundary condition $x_0(t) = 0$, $x_{N+1}(t) = 0$. Here, γ denotes the damping constant, $E_i(t), i = 1, N$ are the random force operators and δ_{ij} is the Kronecker δ. 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, $< E_i(t) >= 0$, and their second moments are determined by the commutator

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

and the symmetrized mean

$$\frac{1}{2} < E_i(t)E_j(s) + E_j(s)E_i(t) >= \delta_{ij}\frac{\gamma}{\pi}\int_0^\infty d\omega\hbar\omega \coth(\frac{\hbar\omega}{2k_BT_i})\cos\omega(t-s). \quad (4)$$

Here, the average $<>$ 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. $< x_n(t)x_m(t) >, < x_n(t)p_m(t) >$, 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 explicitely.

2. Results

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

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

where the quantity δ 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, Θ_D, we find

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

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

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